BUTANOIC ACID, 2-METHYL-, PROPYL ESTER

Other names: n-Propyl 2-methyl butyrate
Propyl 2-methylbutanoate
Propyl 2-methylbutyrate
Inchi: InChI=1S/C8H16O2/c1-4-6-10-8(9)7(3)5-2/h7H,4-6H2,1-3H3
InchiKey: TZFQMSDUSOTCJC-UHFFFAOYSA-N
Formula: C8H16O2
SMILES: CCCOC(=O)C(C)CC
Mol. weight [g/mol]: 144.21

Physical Properties

Property code	Value	Unit	Source
hf	-544.57	kJ/mol	Cheméo Relay (1.0)
hfus	15.74	kJ/mol	Joback Method
hvap	44.00	kJ/mol	Cheméo Relay (1.0)
ie	9.69	eV	Cheméo Relay (1.0)
log10ws	-1.99		Cheméo Relay (1.0)
logp	1.986		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	943.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	944.30		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	947.00		NIST Webbook

ripol	1125.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1136.00		NIST Webbook
ripol	1132.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1094.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1150.00		NIST Webbook
ripol	1134.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1136.00		NIST Webbook
ripol	1125.00		NIST Webbook
ripol	1094.00		NIST Webbook
tb	411.86	K	Cheméo Relay (1.0)
tc	600.55	K	Cheméo Relay (1.0)
tf	197.53	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.83	J/mol×K	458.29	Joback Method
cpg	348.57	J/mol×K	637.16	Joback Method
cpg	338.23	J/mol×K	607.34	Joback Method
cpg	327.44	J/mol×K	577.53	Joback Method
cpg	316.22	J/mol×K	547.72	Joback Method
cpg	304.54	J/mol×K	517.91	Joback Method
cpg	292.41	J/mol×K	488.10	Joback Method
dvisc	0.0006713	Pa×s	347.69	Joback Method
dvisc	0.0002420	Pa×s	458.29	Joback Method
dvisc	0.0003204	Pa×s	421.42	Joback Method
dvisc	0.0004476	Pa×s	384.55	Joback Method
dvisc	0.0048246	Pa×s	237.08	Joback Method
dvisc	0.0011084	Pa×s	310.82	Joback Method
dvisc	0.0020946	Pa×s	273.95	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37064203&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point