Butanoic acid, 2-methyl-, pentyl ester

Other names:	Amyl 2-methylbutyrate
	N-Amyl 2-methyl butyrate
	n-Amyl 2-methylbutanoate
	Pentyl 2-methylbutyrate
	Pentyl 2-methylbutanoate
Inchi:	InChI=1S/C10H20O2/c1-4-6-7-8-12-10(11)9(3)5-2/h9H,4-8H2,1-3H3
InchiKey:	RHNBXPIJLXBHMF-UHFFFAOYSA-N
Formula:	C10H20O2
SMILES:	CCCCCOC(=O)C(C)CC
Mol. weight [g/mol]:	172.26
CAS:	68039-26-9

Physical Properties

Property code	Value	Unit	Source
gf	-203.04	kJ/mol	Joback Method
hf	-499.81	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.766		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	1135.60		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1174.00		NIST Webbook

rinpol	1126.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1324.00		NIST Webbook
ripol	1327.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1316.00		NIST Webbook
tb	504.05	K	Joback Method
tc	679.81	K	Joback Method
tf	259.62	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.31	J/mol×K	504.05	Joback Method
cpg	435.35	J/mol×K	650.52	Joback Method
cpg	423.03	J/mol×K	621.22	Joback Method
cpg	410.17	J/mol×K	591.93	Joback Method
cpg	396.77	J/mol×K	562.64	Joback Method
cpg	382.82	J/mol×K	533.34	Joback Method
cpg	447.14	J/mol×K	679.81	Joback Method
dvisc	0.0002109	Pa×s	504.05	Joback Method
dvisc	0.0002816	Pa×s	463.31	Joback Method
dvisc	0.0003976	Pa×s	422.57	Joback Method
dvisc	0.0006043	Pa×s	381.84	Joback Method
dvisc	0.0010151	Pa×s	341.10	Joback Method
dvisc	0.0019627	Pa×s	300.36	Joback Method
dvisc	0.0046674	Pa×s	259.62	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C68039269&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
vc:	Critical Volume