Pentanoic acid, 2-methyl, 3-methylbutyl ester

Inchi: InChI=1S/C11H22O2/c1-5-6-10(4)11(12)13-8-7-9(2)3/h9-10H,5-8H2,1-4H3
InchiKey: ACBVJQOFOUNQJU-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: CCCC(C)C(=O)OCCC(C)C
Mol. weight [g/mol]: 186.29

Physical Properties

Property code	Value	Unit	Source
gf	-197.06	kJ/mol	Joback Method
hf	-525.73	kJ/mol	Joback Method
hfus	19.99	kJ/mol	Joback Method
hvap	48.46	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	3.012		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	1153.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1153.00		NIST Webbook
tb	526.49	K	Joback Method
tc	704.16	K	Joback Method
tf	255.89	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.72	J/mol×K	526.49	Joback Method
cpg	487.83	J/mol×K	674.54	Joback Method
cpg	474.64	J/mol×K	644.93	Joback Method
cpg	460.84	J/mol×K	615.32	Joback Method
cpg	446.42	J/mol×K	585.71	Joback Method

cpg	431.38	J/mol×K	556.10	Joback Method
cpg	500.43	J/mol×K	704.16	Joback Method
dvisc	0.0001825	Pa×s	526.49	Joback Method
dvisc	0.0002510	Pa×s	481.39	Joback Method
dvisc	0.0003687	Pa×s	436.29	Joback Method
dvisc	0.0005917	Pa×s	391.19	Joback Method
dvisc	0.0010741	Pa×s	346.09	Joback Method
dvisc	0.0023315	Pa×s	300.99	Joback Method
dvisc	0.0066509	Pa×s	255.89	Joback Method

Sources

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=R97367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume