6-Methylheptyl 2-methylbutanoate

Inchi: InChI=1S/C13H26O2/c1-5-12(4)13(14)15-10-8-6-7-9-11(2)3/h11-12H,5-10H2,1-4H3
InchiKey: YNYPOSLGRAFYEW-UHFFFAOYSA-N
Formula: C13H26O2
SMILES: CCC(C)C(=O)OCCCCCC(C)C
Mol. weight [g/mol]: 214.34
CAS: 117421-31-5

Physical Properties

Property code	Value	Unit	Source
gf	-180.22	kJ/mol	Joback Method
hf	-567.01	kJ/mol	Joback Method
hfus	25.17	kJ/mol	Joback Method
hvap	52.91	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.792		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	1397.70		NIST Webbook
rinpol	1397.70		NIST Webbook
tb	572.25	K	Joback Method
tc	746.93	K	Joback Method
tf	278.43	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.40	J/mol×K	572.25	Joback Method
cpg	532.39	J/mol×K	601.36	Joback Method
cpg	548.66	J/mol×K	630.48	Joback Method
cpg	564.24	J/mol×K	659.59	Joback Method
cpg	579.14	J/mol×K	688.70	Joback Method
cpg	593.36	J/mol×K	717.82	Joback Method
cpg	606.91	J/mol×K	746.93	Joback Method

dvisc	0.0057377	Pa×s	278.43	Joback Method
dvisc	0.0019823	Pa×s	327.40	Joback Method
dvisc	0.0009030	Pa×s	376.37	Joback Method
dvisc	0.0004930	Pa×s	425.34	Joback Method
dvisc	0.0003050	Pa×s	474.31	Joback Method
dvisc	0.0002064	Pa×s	523.28	Joback Method
dvisc	0.0001494	Pa×s	572.25	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=C117421315&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