Heptadecanoic acid, isobutyl ester

Other names: Isobutyl heptadecanoate
Inchi: InChI=1S/C21H42O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21(22)23-19-20(2)3/h2
InchiKey: AHJVCLSWNOYFEP-UHFFFAOYSA-N
Formula: C21H42O2
SMILES: CCCCCCCCCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 326.56

Physical Properties

Property code	Value	Unit	Source
gf	-110.42	kJ/mol	Joback Method
hf	-726.85	kJ/mol	Joback Method
hfus	49.41	kJ/mol	Joback Method
hvap	71.11	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	7.057		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	755.73	K	Joback Method
tc	930.28	K	Joback Method
tf	383.59	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.75	J/mol×K	755.73	Joback Method
cpg	989.99	J/mol×K	784.82	Joback Method
cpg	1009.24	J/mol×K	813.91	Joback Method
cpg	1027.53	J/mol×K	843.00	Joback Method
cpg	1044.89	J/mol×K	872.09	Joback Method
cpg	1061.34	J/mol×K	901.19	Joback Method
cpg	1076.91	J/mol×K	930.28	Joback Method

dvisc	0.0018724	Pa×s	383.59	Joback Method
dvisc	0.0007045	Pa×s	445.61	Joback Method
dvisc	0.0003366	Pa×s	507.64	Joback Method
dvisc	0.0001889	Pa×s	569.66	Joback Method
dvisc	0.0001187	Pa×s	631.68	Joback Method
dvisc	0.0000811	Pa×s	693.71	Joback Method
dvisc	0.0000590	Pa×s	755.73	Joback Method

Sources

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=U405167&Units=SI
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
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