Heneicosanoic acid, isobutyl ester

Other names: Isobutyl heneicosanoate
Inchi: InChI=1S/C25H50O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25(26)27
InchiKey: CFKCCHCICMBUPR-UHFFFAOYSA-N
Formula: C25H50O2
SMILES: CCCCCCCCCCCCCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 382.66

Physical Properties

Property code	Value	Unit	Source
gf	-76.74	kJ/mol	Joback Method
hf	-809.41	kJ/mol	Joback Method
hfus	59.77	kJ/mol	Joback Method
hvap	80.01	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	8.617		Crippen Method
mcvol	370.550	ml/mol	McGowan Method
pc	787.27	kPa	Joback Method
rinpol	2634.00		NIST Webbook
tb	847.25	K	Joback Method
tc	1037.37	K	Joback Method
tf	428.67	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1221.19	J/mol×K	847.25	Joback Method
cpg	1320.21	J/mol×K	1005.69	Joback Method
cpg	1302.75	J/mol×K	974.00	Joback Method
cpg	1284.15	J/mol×K	942.31	Joback Method
cpg	1264.39	J/mol×K	910.62	Joback Method
cpg	1243.42	J/mol×K	878.94	Joback Method
cpg	1336.60	J/mol×K	1037.37	Joback Method
dvisc	0.0000331	Pa×s	847.25	Joback Method

dvisc	0.0000458	Pa×s	777.49	Joback Method
dvisc	0.0000676	Pa×s	707.72	Joback Method
dvisc	0.0001086	Pa×s	637.96	Joback Method
dvisc	0.0001961	Pa×s	568.20	Joback Method
dvisc	0.0004178	Pa×s	498.43	Joback Method
dvisc	0.0011387	Pa×s	428.67	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=U405170&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