Docosanoic acid, isobutyl ester

Other names: Isobutyl behenoate
Inchi: InChI=1S/C26H52O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26(27
InchiKey: MLOOWFAQLIBHEP-UHFFFAOYSA-N
Formula: C26H52O2
SMILES: CCCCCCCCCCCCCCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 396.69

Physical Properties

Property code	Value	Unit	Source
gf	-68.32	kJ/mol	Joback Method
hf	-830.05	kJ/mol	Joback Method
hfus	62.36	kJ/mol	Joback Method
hvap	82.24	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	9.008		Crippen Method
mcvol	384.640	ml/mol	McGowan Method
pc	746.51	kPa	Joback Method
rinpol	2724.00		NIST Webbook
rinpol	2724.00		NIST Webbook
tb	870.13	K	Joback Method
tc	1066.30	K	Joback Method
tf	439.94	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1285.77	J/mol×K	870.13	Joback Method
cpg	1308.62	J/mol×K	902.82	Joback Method
cpg	1330.12	J/mol×K	935.52	Joback Method
cpg	1350.31	J/mol×K	968.21	Joback Method
cpg	1369.26	J/mol×K	1000.91	Joback Method
cpg	1387.01	J/mol×K	1033.60	Joback Method
cpg	1403.60	J/mol×K	1066.30	Joback Method

dvisc	0.0009974	Pa×s	439.94	Joback Method
dvisc	0.0003640	Pa×s	511.64	Joback Method
dvisc	0.0001702	Pa×s	583.34	Joback Method
dvisc	0.0000940	Pa×s	655.04	Joback Method
dvisc	0.0000583	Pa×s	726.73	Joback Method
dvisc	0.0000395	Pa×s	798.43	Joback Method
dvisc	0.0000285	Pa×s	870.13	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=U405171&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume