

Cyclopropanetetradecanoic acid, 2-octyl-, methyl ester

Inchi: InChI=1S/C26H50O2/c1-3-4-5-6-14-17-20-24-23-25(24)21-18-15-12-10-8-7-9-11-13-16-19
InchiKey: JBDGXWZXMAXBLS-UHFFFAOYSA-N
Formula: C26H50O2
SMILES: CCCCCCCCC1CC1CCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 394.67
CAS: 52355-42-7

Physical Properties

Property code	Value	Unit	Source
gf	-12.84	kJ/mol	Joback Method
hf	-772.31	kJ/mol	Joback Method
hfus	65.09	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.617		Crippen Method
mcvol	373.780	ml/mol	McGowan Method
pc	784.19	kPa	Joback Method
tb	872.64	K	Joback Method
tc	1068.57	K	Joback Method
tf	468.64	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1272.87	J/mol×K	872.64	Joback Method
cpg	1295.61	J/mol×K	905.30	Joback Method
cpg	1317.08	J/mol×K	937.95	Joback Method
cpg	1337.35	J/mol×K	970.61	Joback Method
cpg	1356.47	J/mol×K	1003.26	Joback Method
cpg	1374.51	J/mol×K	1035.92	Joback Method
cpg	1391.54	J/mol×K	1068.57	Joback Method
dvisc	0.0013190	Pa×s	468.64	Joback Method
dvisc	0.0007000	Pa×s	535.97	Joback Method

dvisc	0.0004279	Pa×s	603.31	Joback Method
dvisc	0.0002888	Pa×s	670.64	Joback Method
dvisc	0.0002094	Pa×s	737.97	Joback Method
dvisc	0.0001602	Pa×s	805.31	Joback Method
dvisc	0.0001277	Pa×s	872.64	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=C52355427&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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