Dimethylmalonic acid, hexyl pentadecyl ester

Inchi: InChI=1S/C26H50O4/c1-5-7-9-11-12-13-14-15-16-17-18-19-21-23-30-25(28)26(3,4)24(2
InchiKey: FNEKWEKLAFXPMK-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCC
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-296.96	kJ/mol	Joback Method
hf	-1078.32	kJ/mol	Joback Method
hfus	61.26	kJ/mol	Joback Method
hvap	90.49	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	7.771		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	770.32	kPa	Joback Method
rinpol	2707.00		NIST Webbook
rinpol	2707.00		NIST Webbook
tb	943.63	K	Joback Method
tc	1158.72	K	Joback Method
tf	529.52	K	Joback Method
vc	1.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.97	J/mol×K	943.63	Joback Method
cpg	1365.90	J/mol×K	979.48	Joback Method
cpg	1385.32	J/mol×K	1015.33	Joback Method
cpg	1403.28	J/mol×K	1051.17	Joback Method
cpg	1419.86	J/mol×K	1087.02	Joback Method
cpg	1435.13	J/mol×K	1122.87	Joback Method
cpg	1449.14	J/mol×K	1158.72	Joback Method
dvisc	0.0003659	Pa×s	529.52	Joback Method

dvisc	0.0001622	Pa×s	598.54	Joback Method
dvisc	0.0000851	Pa×s	667.56	Joback Method
dvisc	0.0000504	Pa×s	736.58	Joback Method
dvisc	0.0000326	Pa×s	805.59	Joback Method
dvisc	0.0000226	Pa×s	874.61	Joback Method
dvisc	0.0000166	Pa×s	943.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361696&Units=SI
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

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