Diethylmalonic acid, hexadecyl 2-methoxyethyl ester

Inchi: InChI=1S/C26H50O5/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-30-24(27)26(6-2,7-
InchiKey: HUAHBJXSROVQFQ-UHFFFAOYSA-N
Formula: C26H50O5
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCOC
Mol. weight [g/mol]: 442.67

Physical Properties

Property code	Value	Unit	Source
gf	-401.96	kJ/mol	Joback Method
hf	-1210.54	kJ/mol	Joback Method
hfus	62.44	kJ/mol	Joback Method
hvap	92.90	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	7.007		Crippen Method
mcvol	397.950	ml/mol	McGowan Method
pc	763.10	kPa	Joback Method
rinpol	2812.00		NIST Webbook
rinpol	2812.00		NIST Webbook
tb	966.05	K	Joback Method
tc	1189.08	K	Joback Method
tf	551.75	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1376.87	J/mol×K	966.05	Joback Method
cpg	1462.80	J/mol×K	1151.91	Joback Method
cpg	1448.85	J/mol×K	1114.73	Joback Method
cpg	1433.34	J/mol×K	1077.56	Joback Method
cpg	1416.21	J/mol×K	1040.39	Joback Method
cpg	1397.41	J/mol×K	1003.22	Joback Method
cpg	1475.24	J/mol×K	1189.08	Joback Method
dvisc	0.0000121	Pa×s	966.05	Joback Method

dvisc	0.0000164	Pa×s	897.00	Joback Method
dvisc	0.0000235	Pa×s	827.95	Joback Method
dvisc	0.0000359	Pa×s	758.90	Joback Method
dvisc	0.0000598	Pa×s	689.85	Joback Method
dvisc	0.0001113	Pa×s	620.80	Joback Method
dvisc	0.0002423	Pa×s	551.75	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=U370683&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