Diethylmalonic acid, decyl hexyl ester

Inchi: InChI=1S/C23H44O4/c1-5-9-11-13-14-15-16-18-20-27-22(25)23(7-3,8-4)21(24)26-19-17-
InchiKey: CHFCJYHIXJKWBL-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCC
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-322.22	kJ/mol	Joback Method
hf	-1016.40	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	83.81	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.600		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	2358.00		NIST Webbook
tb	874.99	K	Joback Method
tc	1071.31	K	Joback Method
tf	495.71	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.79	J/mol×K	874.99	Joback Method
cpg	1174.20	J/mol×K	907.71	Joback Method
cpg	1192.37	J/mol×K	940.43	Joback Method
cpg	1209.35	J/mol×K	973.15	Joback Method
cpg	1225.18	J/mol×K	1005.87	Joback Method
cpg	1239.91	J/mol×K	1038.59	Joback Method
cpg	1253.57	J/mol×K	1071.31	Joback Method
dvisc	0.0005484	Pa×s	495.71	Joback Method
dvisc	0.0002494	Pa×s	558.92	Joback Method

dvisc	0.0001331	Pa×s	622.14	Joback Method
dvisc	0.0000798	Pa×s	685.35	Joback Method
dvisc	0.0000521	Pa×s	748.56	Joback Method
dvisc	0.0000364	Pa×s	811.78	Joback Method
dvisc	0.0000268	Pa×s	874.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369445&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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