

Diethylmalonic acid, hexyl nonyl ester

Inchi:	InChI=1S/C22H42O4/c1-5-9-11-13-14-15-17-19-26-21(24)22(7-3,8-4)20(23)25-18-16-12
InchiKey:	XCDKNOIELATBKD-UHFFFAOYSA-N
Formula:	C22H42O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
Mol. weight [g/mol]:	370.57

Physical Properties

Property code	Value	Unit	Source
gf	-330.64	kJ/mol	Joback Method
hf	-995.76	kJ/mol	Joback Method
hfus	50.90	kJ/mol	Joback Method
hvap	81.58	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	6.210		Crippen Method
mvol	335.720	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	2256.00		NIST Webbook
tb	852.11	K	Joback Method
tc	1044.11	K	Joback Method
tf	484.44	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.56	J/molxK	852.11	Joback Method
cpg	1111.54	J/molxK	884.11	Joback Method
cpg	1129.36	J/molxK	916.11	Joback Method
cpg	1146.06	J/molxK	948.11	Joback Method
cpg	1161.66	J/molxK	980.11	Joback Method
cpg	1176.22	J/molxK	1012.11	Joback Method
cpg	1189.77	J/molxK	1044.11	Joback Method
dvisc	0.0006242	Paxs	484.44	Joback Method
dvisc	0.0002865	Paxs	545.72	Joback Method

dvisc	0.0001539	Paxs	607.00	Joback Method
dvisc	0.0000927	Paxs	668.27	Joback Method
dvisc	0.0000608	Paxs	729.55	Joback Method
dvisc	0.0000425	Paxs	790.83	Joback Method
dvisc	0.0000313	Paxs	852.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U369444&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

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