

Diethylmalonic acid, decyl tetrahydrofurfuryl ester

Inchi:	InChI=1S/C22H40O5/c1-4-7-8-9-10-11-12-13-16-26-20(23)22(5-2,6-3)21(24)27-18-19-15
InchiKey:	BNPDQFIZHQJOHO-UHFFFAOYSA-N
Formula:	C22H40O5
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC1CCCO1
Mol. weight [g/mol]:	384.55

Physical Properties

Property code	Value	Unit	Source
gf	-380.21	kJ/mol	Joback Method
hf	-1067.28	kJ/mol	Joback Method
hfus	52.81	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	5.199		Crippen Method
mvol	330.730	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	894.34	K	Joback Method
tc	1097.66	K	Joback Method
tf	521.91	K	Joback Method
vc	1.266	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.54	J/molxK	894.34	Joback Method
cpg	1138.94	J/molxK	928.23	Joback Method
cpg	1156.03	J/molxK	962.11	Joback Method
cpg	1171.86	J/molxK	996.00	Joback Method
cpg	1186.49	J/molxK	1029.88	Joback Method
cpg	1199.97	J/molxK	1063.77	Joback Method
cpg	1212.34	J/molxK	1097.66	Joback Method
dvisc	0.0006388	Paxs	521.91	Joback Method

dvisc	0.0003134	Paxs	583.98	Joback Method
dvisc	0.0001763	Paxs	646.05	Joback Method
dvisc	0.0001097	Paxs	708.12	Joback Method
dvisc	0.0000737	Paxs	770.20	Joback Method
dvisc	0.0000525	Paxs	832.27	Joback Method
dvisc	0.0000392	Paxs	894.34	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=U370645&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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