

Diethylmalonic acid, dodecyl tetrahydrofurfuryl ester

Inchi:	InChI=1S/C24H44O5/c1-4-7-8-9-10-11-12-13-14-15-18-28-22(25)24(5-2,6-3)23(26)29-20
InchiKey:	HDSMWCSOUVPZAB-UHFFFAOYSA-N
Formula:	C24H44O5
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC1CCCO1
Mol. weight [g/mol]:	412.60

Physical Properties

Property code	Value	Unit	Source
gf	-363.37	kJ/mol	Joback Method
hf	-1108.56	kJ/mol	Joback Method
hfus	57.99	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.979		Crippen Method
mcvol	358.910	ml/mol	McGowan Method
pc	952.60	kPa	Joback Method
rinpol	2664.00		NIST Webbook
tb	940.10	K	Joback Method
tc	1151.02	K	Joback Method
tf	544.45	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1245.49	J/molxK	940.10	Joback Method
cpg	1264.39	J/molxK	975.25	Joback Method
cpg	1281.86	J/molxK	1010.41	Joback Method
cpg	1297.97	J/molxK	1045.56	Joback Method
cpg	1312.78	J/molxK	1080.71	Joback Method
cpg	1326.35	J/molxK	1115.87	Joback Method
cpg	1338.76	J/molxK	1151.02	Joback Method
dvisc	0.0004930	Paxs	544.45	Joback Method
dvisc	0.0002373	Paxs	610.39	Joback Method

dvisc	0.0001317	Paxs	676.33	Joback Method
dvisc	0.0000812	Paxs	742.27	Joback Method
dvisc	0.0000541	Paxs	808.22	Joback Method
dvisc	0.0000384	Paxs	874.16	Joback Method
dvisc	0.0000286	Paxs	940.10	Joback Method

Sources

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=U370647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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