

Diethylmalonic acid, dodecyl 2-ethoxylethyl ester

Inchi:	InChI=1S/C23H44O5/c1-5-9-10-11-12-13-14-15-16-17-18-27-21(24)23(6-2,7-3)22(25)28
InchiKey:	JKXJMHTWXWRRMB-UHFFFAOYSA-N
Formula:	C23H44O5
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCOCC
Mol. weight [g/mol]:	400.59

Physical Properties

Property code	Value	Unit	Source
gf	-427.22	kJ/mol	Joback Method
hf	-1148.62	kJ/mol	Joback Method
hfus	54.67	kJ/mol	Joback Method
hvap	86.22	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.837		Crippen Method
mcvol	355.680	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	2442.00		NIST Webbook
tb	897.41	K	Joback Method
tc	1098.80	K	Joback Method
tf	517.94	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.80	J/molxK	897.41	Joback Method
cpg	1205.89	J/molxK	930.98	Joback Method
cpg	1223.63	J/molxK	964.54	Joback Method
cpg	1240.04	J/molxK	998.11	Joback Method
cpg	1255.15	J/molxK	1031.67	Joback Method
cpg	1269.01	J/molxK	1065.24	Joback Method
cpg	1281.64	J/molxK	1098.80	Joback Method
dvisc	0.0003645	Paxs	517.94	Joback Method
dvisc	0.0001720	Paxs	581.19	Joback Method

dvisc	0.0000940	Paxs	644.43	Joback Method
dvisc	0.0000573	Paxs	707.67	Joback Method
dvisc	0.0000378	Paxs	770.92	Joback Method
dvisc	0.0000266	Paxs	834.16	Joback Method
dvisc	0.0000197	Paxs	897.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370613&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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