

Diethylmalonic acid, ethyl hexyl ester

Inchi:	InChI=1S/C15H28O4/c1-5-9-10-11-12-19-14(17)15(6-2,7-3)13(16)18-8-4/h5-12H2,1-4H3
InchiKey:	JVKSOZUUKCRFAC-UHFFFAOYSA-N
Formula:	C15H28O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OCC
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
gf	-389.58	kJ/mol	Joback Method
hf	-851.28	kJ/mol	Joback Method
hfus	32.77	kJ/mol	Joback Method
hvap	66.00	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.479		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	1607.00		NIST Webbook
tb	691.95	K	Joback Method
tc	874.06	K	Joback Method
tf	405.55	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.64	J/molxK	691.95	Joback Method
cpg	696.12	J/molxK	722.30	Joback Method
cpg	711.75	J/molxK	752.65	Joback Method
cpg	726.55	J/molxK	783.00	Joback Method
cpg	740.53	J/molxK	813.36	Joback Method
cpg	753.71	J/molxK	843.71	Joback Method
cpg	766.12	J/molxK	874.06	Joback Method
dvisc	0.0014014	Paxs	405.55	Joback Method
dvisc	0.0006952	Paxs	453.28	Joback Method

dvisc	0.0003941	Paxs	501.02	Joback Method
dvisc	0.0002466	Paxs	548.75	Joback Method
dvisc	0.0001664	Paxs	596.48	Joback Method
dvisc	0.0001190	Paxs	644.22	Joback Method
dvisc	0.0000891	Paxs	691.95	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=U369437&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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