

Diethylmalonic acid, di(2-ethoxyethyl) ester

Inchi:	InChI=1S/C15H28O6/c1-5-15(6-2,13(16)20-11-9-18-7-3)14(17)21-12-10-19-8-4/h5-12H2
InchiKey:	JBHBIXWXJITXLE-UHFFFAOYSA-N
Formula:	C15H28O6
SMILES:	CCOCCOC(=O)C(CC)(CC)C(=O)OCCOCC
Mol. weight [g/mol]:	304.38

Physical Properties

Property code	Value	Unit	Source
gf	-599.58	kJ/mol	Joback Method
hf	-1115.72	kJ/mol	Joback Method
hfus	35.14	kJ/mol	Joback Method
hvap	70.82	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.952		Crippen Method
mcvol	248.830	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinqol	1743.00		NIST Webbook
tb	736.79	K	Joback Method
tc	919.63	K	Joback Method
tf	450.01	K	Joback Method
vc	0.949	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.23	J/molxK	736.79	Joback Method
cpg	809.09	J/molxK	889.16	Joback Method
cpg	796.69	J/molxK	858.68	Joback Method
cpg	783.41	J/molxK	828.21	Joback Method
cpg	769.24	J/molxK	797.74	Joback Method
cpg	754.18	J/molxK	767.26	Joback Method
cpg	820.60	J/molxK	919.63	Joback Method
dvisc	0.0000505	Paxs	736.79	Joback Method
dvisc	0.0000667	Paxs	688.99	Joback Method

dvisc	0.0000917	Paxs	641.20	Joback Method
dvisc	0.0001327	Paxs	593.40	Joback Method
dvisc	0.0002050	Paxs	545.60	Joback Method
dvisc	0.0003441	Paxs	497.81	Joback Method
dvisc	0.0006449	Paxs	450.01	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=U370618&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
mccvol:	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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