

Diethylmalonic acid, ethyl isopropyl ester

Inchi:	InChI=1S/C12H22O4/c1-6-12(7-2,10(13)15-8-3)11(14)16-9(4)5/h9H,6-8H2,1-5H3
InchiKey:	ZXADVZIAXXDCRH-UHFFFAOYSA-N
Formula:	C12H22O4
SMILES:	CCOC(=O)C(CC)(CC)C(=O)OC(C)C
Mol. weight [g/mol]:	230.30

Physical Properties

Property code	Value	Unit	Source
gf	-417.28	kJ/mol	Joback Method
hf	-794.64	kJ/mol	Joback Method
hfus	21.47	kJ/mol	Joback Method
hvap	58.93	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.308		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	1260.00		NIST Webbook
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tb	622.87	K	Joback Method
tc	811.82	K	Joback Method
tf	356.74	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.38	J/molxK	622.87	Joback Method
cpg	588.77	J/molxK	780.32	Joback Method
cpg	576.41	J/molxK	748.83	Joback Method
cpg	563.30	J/molxK	717.34	Joback Method
cpg	549.44	J/molxK	685.85	Joback Method
cpg	534.80	J/molxK	654.36	Joback Method
cpg	600.40	J/molxK	811.82	Joback Method
dvisc	0.0001246	Paxs	622.87	Joback Method

dvisc	0.0001685	Paxs	578.51	Joback Method
dvisc	0.0002397	Paxs	534.16	Joback Method
dvisc	0.0003635	Paxs	489.81	Joback Method
dvisc	0.0005987	Paxs	445.45	Joback Method
dvisc	0.0011014	Paxs	401.10	Joback Method
dvisc	0.0023577	Paxs	356.74	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=U370261&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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