

Diethylmalonic acid, ethyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C15H28O4/c1-7-15(8-2,13(16)18-9-3)14(17)19-12(6)10-11(4)5/h11-12H,7-10H
InchiKey:	QOMKEPLQRXPOCG-UHFFFAOYSA-N
Formula:	C15H28O4
SMILES:	CCOC(=O)C(CC)(CC)C(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
gf	-394.46	kJ/mol	Joback Method
hf	-861.84	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	65.22	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.334		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
rinpol	1472.00		NIST Webbook
tb	691.07	K	Joback Method
tc	878.32	K	Joback Method
tf	375.55	K	Joback Method
vc	0.900	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.58	J/molxK	691.07	Joback Method
cpg	697.58	J/molxK	722.28	Joback Method
cpg	713.66	J/molxK	753.49	Joback Method
cpg	728.85	J/molxK	784.70	Joback Method
cpg	743.16	J/molxK	815.90	Joback Method
cpg	756.61	J/molxK	847.11	Joback Method
cpg	769.22	J/molxK	878.32	Joback Method
dvisc	0.0022315	Paxs	375.55	Joback Method
dvisc	0.0009002	Paxs	428.14	Joback Method

dvisc	0.0004430	Paxs	480.72	Joback Method
dvisc	0.0002507	Paxs	533.31	Joback Method
dvisc	0.0001571	Paxs	585.90	Joback Method
dvisc	0.0001064	Paxs	638.48	Joback Method
dvisc	0.0000764	Paxs	691.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370493&Units=SI
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

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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