

Diethylmalonic acid, 3-methylbutyl propyl ester

Inchi: InChI=1S/C15H28O4/c1-6-10-18-13(16)15(7-2,8-3)14(17)19-11-9-12(4)5/h12H,6-11H2,1H3
InchiKey: LBCMESLETWPRCF-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CCCOC(=O)C(CC)(CC)C(=O)OCCC(C)C
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-392.02	kJ/mol	Joback Method
hf	-856.56	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	65.61	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.335		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	1551.00		NIST Webbook
tb	691.51	K	Joback Method
tc	876.12	K	Joback Method
tf	390.55	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.11	J/molxK	691.51	Joback Method
cpg	755.14	J/molxK	845.35	Joback Method
cpg	741.83	J/molxK	814.59	Joback Method
cpg	727.68	J/molxK	783.82	Joback Method
cpg	712.70	J/molxK	753.05	Joback Method
cpg	696.84	J/molxK	722.28	Joback Method
cpg	767.65	J/molxK	876.12	Joback Method
dvisc	0.0000825	Paxs	691.51	Joback Method
dvisc	0.0001124	Paxs	641.35	Joback Method

dvisc	0.0001615	Paxs	591.19	Joback Method
dvisc	0.0002481	Paxs	541.03	Joback Method
dvisc	0.0004162	Paxs	490.87	Joback Method
dvisc	0.0007852	Paxs	440.71	Joback Method
dvisc	0.0017437	Paxs	390.55	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=U369382&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
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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