

Diethylmalonic acid, isobutyl 5-methylhex-2-yl ester

Inchi:	InChI=1S/C18H34O4/c1-8-18(9-2,16(19)21-12-14(5)6)17(20)22-15(7)11-10-13(3)4/h13-1
InchiKey:	JRKBKQYGSHWCFH-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCC(CC)(C(=O)OCC(C)C)C(=O)OC(C)CCC(C)C
Mol. weight [g/mol]:	314.46

Physical Properties

Property code	Value	Unit	Source
gf	-371.64	kJ/mol	Joback Method
hf	-929.04	kJ/mol	Joback Method
hfus	29.97	kJ/mol	Joback Method
hvap	71.51	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.360		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1265.55	kPa	Joback Method
rinsol	1760.00		NIST Webbook
tb	759.27	K	Joback Method
tc	947.34	K	Joback Method
tf	394.36	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.50	J/molxK	759.27	Joback Method
cpg	932.87	J/molxK	915.99	Joback Method
cpg	918.78	J/molxK	884.65	Joback Method
cpg	903.72	J/molxK	853.30	Joback Method
cpg	887.68	J/molxK	821.96	Joback Method
cpg	870.61	J/molxK	790.61	Joback Method
cpg	946.02	J/molxK	947.34	Joback Method
dvisc	0.0000451	Paxs	759.27	Joback Method
dvisc	0.0000644	Paxs	698.45	Joback Method

dvisc	0.0000983	Paxs	637.63	Joback Method
dvisc	0.0001640	Paxs	576.82	Joback Method
dvisc	0.0003086	Paxs	516.00	Joback Method
dvisc	0.0006880	Paxs	455.18	Joback Method
dvisc	0.0019641	Paxs	394.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369296&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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