

Diethylmalonic acid, isobutyl 5-methoxy-3-methylpentyl ester

Inchi:	InChI=1S/C18H34O5/c1-7-18(8-2,17(20)23-13-14(3)4)16(19)22-12-10-15(5)9-11-21-6/h1
InchiKey:	YYOBIYGUNGANTN-UHFFFAOYSA-N
Formula:	C18H34O5
SMILES:	CCC(CC)(C(=O)OCCCC(C)CCOC)C(=O)OCC(C)C
Mol. weight [g/mol]:	330.46

Physical Properties

Property code	Value	Unit	Source
gf	-474.20	kJ/mol	Joback Method
hf	-1055.98	kJ/mol	Joback Method
hfus	34.68	kJ/mol	Joback Method
hvap	74.31	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.598		Crippen Method
mcvol	285.230	ml/mol	McGowan Method
pc	1243.33	kPa	Joback Method
rinsol	1897.00		NIST Webbook
tb	782.13	K	Joback Method
tc	969.34	K	Joback Method
tf	431.59	K	Joback Method
vc	1.087	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.81	J/molxK	782.13	Joback Method
cpg	900.38	J/molxK	813.33	Joback Method
cpg	916.89	J/molxK	844.53	Joback Method
cpg	932.36	J/molxK	875.74	Joback Method
cpg	946.82	J/molxK	906.94	Joback Method
cpg	960.27	J/molxK	938.14	Joback Method
cpg	972.74	J/molxK	969.34	Joback Method
dvisc	0.0009908	Paxs	431.59	Joback Method
dvisc	0.0004116	Paxs	490.01	Joback Method

dvisc	0.0002061	Paxs	548.44	Joback Method
dvisc	0.0001180	Paxs	606.86	Joback Method
dvisc	0.0000745	Paxs	665.28	Joback Method
dvisc	0.0000506	Paxs	723.71	Joback Method
dvisc	0.0000365	Paxs	782.13	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=U370763&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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