

Diethylmalonic acid, hexyl tetrahydrofurfuryl ester

Inchi:	InChI=1S/C18H32O5/c1-4-7-8-9-12-22-16(19)18(5-2,6-3)17(20)23-14-15-11-10-13-21-15
InchiKey:	GLEWGPZZFPUAAP-UHFFFAOYSA-N
Formula:	C18H32O5
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OCC1CCCO1
Mol. weight [g/mol]:	328.44

Physical Properties

Property code	Value	Unit	Source
gf	-413.89	kJ/mol	Joback Method
hf	-984.72	kJ/mol	Joback Method
hfus	42.45	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.639		Crippen Method
mvol	274.370	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	2063.00		NIST Webbook
tb	802.82	K	Joback Method
tc	1000.73	K	Joback Method
tf	476.83	K	Joback Method
vc	1.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.06	J/molxK	802.82	Joback Method
cpg	955.29	J/molxK	967.74	Joback Method
cpg	942.02	J/molxK	934.76	Joback Method
cpg	927.70	J/molxK	901.77	Joback Method
cpg	912.29	J/molxK	868.79	Joback Method
cpg	895.76	J/molxK	835.80	Joback Method
cpg	967.55	J/molxK	1000.73	Joback Method
dvisc	0.0000726	Paxs	802.82	Joback Method
dvisc	0.0000962	Paxs	748.49	Joback Method

dvisc	0.0001333	Paxs	694.16	Joback Method
dvisc	0.0001953	Paxs	639.82	Joback Method
dvisc	0.0003071	Paxs	585.49	Joback Method
dvisc	0.0005296	Paxs	531.16	Joback Method
dvisc	0.0010343	Paxs	476.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370641&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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