

Diethylmalonic acid, heptyl pentyl ester

Inchi:	InChI=1S/C19H36O4/c1-5-9-11-12-14-16-23-18(21)19(7-3,8-4)17(20)22-15-13-10-6-2/h5
InchiKey:	QFLFECFAEVSXGQ-UHFFFAOYSA-N
Formula:	C19H36O4
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
Mol. weight [g/mol]:	328.49

Physical Properties

Property code	Value	Unit	Source
gf	-355.90	kJ/mol	Joback Method
hf	-933.84	kJ/mol	Joback Method
hfus	43.13	kJ/mol	Joback Method
hvap	74.90	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.040		Crippen Method
mvol	293.450	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	783.47	K	Joback Method
tc	967.35	K	Joback Method
tf	450.63	K	Joback Method
vc	1.137	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.17	J/molxK	783.47	Joback Method
cpg	989.85	J/molxK	936.70	Joback Method
cpg	975.81	J/molxK	906.05	Joback Method
cpg	960.85	J/molxK	875.41	Joback Method
cpg	944.94	J/molxK	844.76	Joback Method
cpg	928.06	J/molxK	814.12	Joback Method
cpg	1003.00	J/molxK	967.35	Joback Method
dvisc	0.0000497	Paxs	783.47	Joback Method

dvisc	0.0000670	Paxs	728.00	Joback Method
dvisc	0.0000950	Paxs	672.52	Joback Method
dvisc	0.0001433	Paxs	617.05	Joback Method
dvisc	0.0002345	Paxs	561.58	Joback Method
dvisc	0.0004275	Paxs	506.10	Joback Method
dvisc	0.0009035	Paxs	450.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369515&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
mccvol:	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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