

Diethylmalonic acid, heptyl hexyl ester

Inchi:	InChI=1S/C20H38O4/c1-5-9-11-13-15-17-24-19(22)20(7-3,8-4)18(21)23-16-14-12-10-6-2
InchiKey:	NLMAQFCLMPPXCF-UHFFFAOYSA-N
Formula:	C20H38O4
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
Mol. weight [g/mol]:	342.51

Physical Properties

Property code	Value	Unit	Source
gf	-347.48	kJ/mol	Joback Method
hf	-954.48	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	77.13	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.430		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinqol	2061.00		NIST Webbook
tb	806.35	K	Joback Method
tc	992.19	K	Joback Method
tf	461.90	K	Joback Method
vc	1.192	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.19	J/molxK	806.35	Joback Method
cpg	988.42	J/molxK	837.32	Joback Method
cpg	1005.60	J/molxK	868.30	Joback Method
cpg	1021.76	J/molxK	899.27	Joback Method
cpg	1036.94	J/molxK	930.24	Joback Method
cpg	1051.16	J/molxK	961.22	Joback Method
cpg	1064.44	J/molxK	992.19	Joback Method
dvisc	0.0008014	Paxs	461.90	Joback Method
dvisc	0.0003752	Paxs	519.31	Joback Method

dvisc	0.0002043	Paxs	576.72	Joback Method
dvisc	0.0001242	Paxs	634.12	Joback Method
dvisc	0.0000820	Paxs	691.53	Joback Method
dvisc	0.0000577	Paxs	748.94	Joback Method
dvisc	0.0000427	Paxs	806.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369442&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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