

Diethylmalonic acid, 4-chlorophenyl hexyl ester

Inchi:	InChI=1S/C19H27ClO4/c1-4-7-8-9-14-23-17(21)19(5-2,6-3)18(22)24-16-12-10-15(20)11-
InchiKey:	LQPSHXYGDAATTQC-UHFFFAOYSA-N
Formula:	C19H27ClO4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	354.87

Physical Properties

Property code	Value	Unit	Source
gf	-265.05	kJ/mol	Joback Method
hf	-724.52	kJ/mol	Joback Method
hfus	40.97	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.175		Crippen Method
mvol	281.930	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	2213.00		NIST Webbook
tb	852.56	K	Joback Method
tc	1062.41	K	Joback Method
tf	519.49	K	Joback Method
vc	1.077	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.32	J/molxK	852.56	Joback Method
cpg	862.22	J/molxK	887.53	Joback Method
cpg	876.01	J/molxK	922.51	Joback Method
cpg	888.71	J/molxK	957.48	Joback Method
cpg	900.38	J/molxK	992.46	Joback Method
cpg	911.06	J/molxK	1027.43	Joback Method
cpg	920.80	J/molxK	1062.41	Joback Method
dvisc	0.0004879	Paxs	519.49	Joback Method
dvisc	0.0002677	Paxs	575.00	Joback Method

dvisc	0.0001632	Paxs	630.51	Joback Method
dvisc	0.0001078	Paxs	686.02	Joback Method
dvisc	0.0000758	Paxs	741.54	Joback Method
dvisc	0.0000560	Paxs	797.05	Joback Method
dvisc	0.0000430	Paxs	852.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369896&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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