

Diethylmalonic acid, 3-chlorobenzyl hexyl ester

Inchi:	InChI=1S/C20H29ClO4/c1-4-7-8-9-13-24-18(22)20(5-2,6-3)19(23)25-15-16-11-10-12-17
InchiKey:	LTEYYOARQYIPLI-UHFFFAOYSA-N
Formula:	C20H29ClO4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Cl)c1
Mol. weight [g/mol]:	368.89

Physical Properties

Property code	Value	Unit	Source
gf	-256.63	kJ/mol	Joback Method
hf	-745.16	kJ/mol	Joback Method
hfus	43.56	kJ/mol	Joback Method
hvap	84.45	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.313		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
rinsol	2349.00		NIST Webbook
tb	875.44	K	Joback Method
tc	1085.28	K	Joback Method
tf	530.76	K	Joback Method
vc	1.133	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.75	J/molxK	875.44	Joback Method
cpg	970.18	J/molxK	1050.31	Joback Method
cpg	959.40	J/molxK	1015.34	Joback Method
cpg	947.61	J/molxK	980.36	Joback Method
cpg	934.77	J/molxK	945.39	Joback Method
cpg	920.83	J/molxK	910.41	Joback Method
cpg	980.01	J/molxK	1085.28	Joback Method
dvisc	0.0000369	Paxs	875.44	Joback Method
dvisc	0.0000482	Paxs	817.99	Joback Method

dvisc	0.0000656	Paxs	760.55	Joback Method
dvisc	0.0000937	Paxs	703.10	Joback Method
dvisc	0.0001427	Paxs	645.65	Joback Method
dvisc	0.0002359	Paxs	588.21	Joback Method
dvisc	0.0004349	Paxs	530.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369346&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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