Diethylmalonic acid, 3-chlorobenzyl pentyl ester

Inchi: InChI=1S/C19H27ClO4/c1-4-7-8-12-23-17(21)19(5-2,6-3)18(22)24-14-15-10-9-11-16(20)

InchiKey: DCEUOJMFLOERNY-UHFFFAOYSA-N

Formula: C19H27ClO4

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Cl)c1

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	-5.54		Crippen Method
logp	4.923		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	2256.00		NIST Webbook
tb	852.56	K	Joback Method
tc	1062.41	K	Joback Method
tf	519.49	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.32	J/mol×K	852.56	Joback Method
cpg	911.06	J/mol×K	1027.43	Joback Method
cpg	900.38	J/mol×K	992.46	Joback Method
cpg	888.71	J/mol×K	957.48	Joback Method
cpg	876.01	J/mol×K	922.51	Joback Method
cpg	862.22	J/mol×K	887.53	Joback Method
cpg	920.80	J/mol×K	1062.41	Joback Method
dvisc	0.0000430	Pa×s	852.56	Joback Method
dvisc	0.0000560	Pa×s	797.05	Joback Method

dvisc	0.0000758	Pa×s	741.54	Joback Method
dvisc	0.0001078	Pa×s	686.02	Joback Method
dvisc	0.0001632	Pa×s	630.51	Joback Method
dvisc	0.0002677	Pa×s	575.00	Joback Method
dvisc	0.0004879	Pa×s	519.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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