Diethylmalonic acid, 3-chlorobenzyl isobutyl ester

Inchi: InChI=1S/C18H25ClO4/c1-5-18(6-2,16(20)22-11-13(3)4)17(21)23-12-14-8-7-9-15(19)10-

InchiKey: FIVXLFLYVNFMBI-UHFFFAOYSA-N

Formula: C18H25ClO4

SMILES: CCC(CC)(C(=O)OCc1cccc(Cl)c1)C(=O)OCC(C)C

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
gf	-275.91	kJ/mol	Joback Method
hf	-709.16	kJ/mol	Joback Method
hfus	34.86	kJ/mol	Joback Method
hvap	79.61	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.389		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
tb	829.24	K	Joback Method
tc	1042.39	K	Joback Method
tf	493.22	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.24	J/mol×K	829.24	Joback Method
cpg	853.68	J/mol×K	1006.86	Joback Method
cpg	843.10	J/mol×K	971.34	Joback Method
cpg	831.50	J/mol×K	935.81	Joback Method
cpg	818.86	J/mol×K	900.29	Joback Method
cpg	805.12	J/mol×K	864.76	Joback Method
cpg	863.30	J/mol×K	1042.39	Joback Method
dvisc	0.0000458	Pa×s	829.24	Joback Method

dvisc	0.0000604	Pa×s	773.24	Joback Method
dvisc	0.0000833	Pa×s	717.23	Joback Method
dvisc	0.0001211	Pa×s	661.23	Joback Method
dvisc	0.0001888	Pa×s	605.23	Joback Method
dvisc	0.0003223	Pa×s	549.22	Joback Method
dvisc	0.0006212	Pa×s	493.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369343&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