

Diethylmalonic acid, 4-chlorobenzyl isobutyl ester

Inchi:	InChI=1S/C18H25ClO4/c1-5-18(6-2,16(20)22-11-13(3)4)17(21)23-12-14-7-9-15(19)10-8
InchiKey:	WJYIIZVVQAGCKC-UHFFFAOYSA-N
Formula:	C18H25ClO4
SMILES:	CCC(CC)(C(=O)OCc1ccc(Cl)cc1)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
rinsol	2125.00		NIST Webbook
tb	829.24	K	Joback Method
tc	1042.39	K	Joback Method
tf	493.22	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.24	J/molxK	829.24	Joback Method
cpg	805.12	J/molxK	864.76	Joback Method
cpg	818.86	J/molxK	900.29	Joback Method
cpg	831.50	J/molxK	935.81	Joback Method
cpg	843.10	J/molxK	971.34	Joback Method
cpg	853.68	J/molxK	1006.86	Joback Method
cpg	863.30	J/molxK	1042.39	Joback Method
dvisc	0.0006212	Paxs	493.22	Joback Method
dvisc	0.0003223	Paxs	549.22	Joback Method

dvisc	0.0001888	Paxs	605.23	Joback Method
dvisc	0.0001211	Paxs	661.23	Joback Method
dvisc	0.0000833	Paxs	717.23	Joback Method
dvisc	0.0000604	Paxs	773.24	Joback Method
dvisc	0.0000458	Paxs	829.24	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369776&Units=SI

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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