

Diethylmalonic acid, butyl 4-chlorobenzyl ester

Inchi:	InChI=1S/C18H25ClO4/c1-4-7-12-22-16(20)18(5-2,6-3)17(21)23-13-14-8-10-15(19)11-9
InchiKey:	REJURUCGLBPJGE-UHFFFAOYSA-N
Formula:	C18H25ClO4
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	340.84

Physical Properties

Property code	Value	Unit	Source
gf	-273.47	kJ/mol	Joback Method
hf	-703.88	kJ/mol	Joback Method
hfus	38.38	kJ/mol	Joback Method
hvap	80.00	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.533		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinsol	2166.00		NIST Webbook
tb	829.68	K	Joback Method
tc	1040.23	K	Joback Method
tf	508.22	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.69	J/molxK	829.68	Joback Method
cpg	852.66	J/molxK	1005.13	Joback Method
cpg	842.10	J/molxK	970.04	Joback Method
cpg	830.56	J/molxK	934.95	Joback Method
cpg	818.01	J/molxK	899.86	Joback Method
cpg	804.40	J/molxK	864.77	Joback Method
cpg	862.29	J/molxK	1040.23	Joback Method
dvisc	0.0000499	Paxs	829.68	Joback Method
dvisc	0.0000648	Paxs	776.10	Joback Method

dvisc	0.0000875	Paxs	722.53	Joback Method
dvisc	0.0001238	Paxs	668.95	Joback Method
dvisc	0.0001862	Paxs	615.37	Joback Method
dvisc	0.0003027	Paxs	561.80	Joback Method
dvisc	0.0005453	Paxs	508.22	Joback Method

Sources

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=U369777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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