

1,3-Bis(4-chlorophenyl)-1-butanone

Inchi:	InChI=1S/C16H14Cl2O/c1-11(12-2-6-14(17)7-3-12)10-16(19)13-4-8-15(18)9-5-13/h2-9,1
InchiKey:	UORMYKLQVWZZHA-UHFFFAOYSA-N
Formula:	C16H14Cl2O
SMILES:	CC(CC(=O)c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	293.19
CAS:	66799-44-8

Physical Properties

Property code	Value	Unit	Source
gf	134.18	kJ/mol	Joback Method
hf	-72.79	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	72.21	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.370		Crippen Method
mcvol	214.830	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
tb	757.09	K	Joback Method
tc	1004.56	K	Joback Method
tf	442.73	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.54	J/molxK	757.09	Joback Method
cpg	555.43	J/molxK	798.33	Joback Method
cpg	568.13	J/molxK	839.58	Joback Method
cpg	579.72	J/molxK	880.82	Joback Method
cpg	590.29	J/molxK	922.07	Joback Method
cpg	599.92	J/molxK	963.31	Joback Method
cpg	608.68	J/molxK	1004.56	Joback Method
dvisc	0.0011601	Paxs	442.73	Joback Method
dvisc	0.0006524	Paxs	495.12	Joback Method

dvisc	0.0004097	Paxs	547.52	Joback Method
dvisc	0.0002790	Paxs	599.91	Joback Method
dvisc	0.0002021	Paxs	652.30	Joback Method
dvisc	0.0001536	Paxs	704.70	Joback Method
dvisc	0.0001213	Paxs	757.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66799448&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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