5-chloro-2-(2-propinyl)benzophenone (CPB)

Inchi: InChI=1S/C16H11ClO/c1-2-6-12-9-10-14(17)11-15(12)16(18)13-7-4-3-5-8-13/h1,3-5,7-11
InchiKey: XMFRKUFYNHJLKS-UHFFFAOYSA-N
Formula: C16H11ClO
SMILES: C#CCc1ccc(Cl)cc1C(=O)c1ccccc1
Mol. weight [g/mol]: 254.71

Physical Properties

Property code	Value	Unit	Source
gf	371.62	kJ/mol	Joback Method
hf	240.13	kJ/mol	Joback Method
hfus	33.27	kJ/mol	Joback Method
hvap	68.08	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	3.747		Crippen Method
mcvol	193.990	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook
tb	710.22	K	Joback Method
tc	967.48	K	Joback Method
tf	474.78	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.58	J/mol×K	710.22	Joback Method
cpg	482.33	J/mol×K	753.10	Joback Method
cpg	494.89	J/mol×K	795.97	Joback Method
cpg	506.35	J/mol×K	838.85	Joback Method
cpg	516.82	J/mol×K	881.73	Joback Method
cpg	526.37	J/mol×K	924.60	Joback Method
cpg	535.11	J/mol×K	967.48	Joback Method

Sources

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=R522279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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