3,4-Dioxymethylenebenzylidene-p-chlorophenylac

Inchi: InChI=1S/C16H10ClNO2/c17-14-4-2-12(3-5-14)13(9-18)7-11-1-6-15-16(8-11)20-10-19-1
InchiKey: DLQRXFJDEIGQFF-NTUHNPAUSA-N
Formula: C16H10ClNO2
SMILES: N#CC(=Cc1ccc2c(c1)OCO2)c1ccc(Cl)cc1
Mol. weight [g/mol]: 283.71
CAS: 104089-74-9

Physical Properties

Property code	Value	Unit	Source
gf	368.91	kJ/mol	Joback Method
hf	150.79	kJ/mol	Joback Method
hfus	41.73	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.133		Crippen Method
mcvol	198.980	ml/mol	McGowan Method
pc	2507.52	kPa	Joback Method
tb	842.64	K	Joback Method
tc	1109.41	K	Joback Method
tf	511.67	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.31	J/mol×K	842.64	Joback Method
cpg	539.40	J/mol×K	887.10	Joback Method
cpg	549.75	J/mol×K	931.56	Joback Method
cpg	559.53	J/mol×K	976.02	Joback Method
cpg	568.91	J/mol×K	1020.48	Joback Method
cpg	578.06	J/mol×K	1064.94	Joback Method
cpg	587.14	J/mol×K	1109.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104089749&Units=SI

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