Buclizine M (hydroxy-chlorobenzophenone), isomer 1, acetylated

Inchi: InChI=1S/C15H11ClO3/c1-10(17)19-14-5-3-2-4-13(14)15(18)11-6-8-12(16)9-7-11/h2-9H

InchiKey: JPDVONYBLNNEPR-UHFFFAOYSA-N

Formula: C15H11ClO3

SMILES: CC(=O)Oc1ccccc1C(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 274.70

Physical Properties

Property code	Value	Unit	Source
gf	-93.79	kJ/mol	Joback Method
hf	-275.93	kJ/mol	Joback Method
hfus	30.49	kJ/mol	Joback Method
hvap	75.15	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.496		Crippen Method
mcvol	195.940	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	773.51	K	Joback Method
tc	1020.33	K	Joback Method
tf	488.70	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.21	J/mol×K	773.51	Joback Method
cpg	513.41	J/mol×K	814.65	Joback Method
cpg	524.47	J/mol×K	855.78	Joback Method
cpg	534.43	J/mol×K	896.92	Joback Method
cpg	543.34	J/mol×K	938.06	Joback Method
cpg	551.24	J/mol×K	979.19	Joback Method

cpg	558.18	J/mol×K	1020.33	Joback Method
dvisc	0.0008144	Pa×s	488.70	Joback Method
dvisc	0.0005203	Pa×s	536.17	Joback Method
dvisc	0.0003576	Pa×s	583.64	Joback Method
dvisc	0.0002600	Pa×s	631.11	Joback Method
dvisc	0.0001977	Pa×s	678.57	Joback Method
dvisc	0.0001558	Pa×s	726.04	Joback Method
dvisc	0.0001264	Pa×s	773.51	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=R536104&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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