Buclizine M (hydroxy-chlorobenzophenone), isomer 2, acetylated

Inchi: InChI=1S/C15H11ClO3/c1-10(17)19-14-8-4-12(5-9-14)15(18)11-2-6-13(16)7-3-11/h2-9H
InchiKey: HCGHXQWZYOHIRH-UHFFFAOYSA-N
Formula: C15H11ClO3
SMILES: CC(=O)Oc1ccc(C(=O)c2ccc(Cl)cc2)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	2230.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2230.00		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	551.24	J/mol×K	979.19	Joback Method
cpg	543.34	J/mol×K	938.06	Joback Method
cpg	534.43	J/mol×K	896.92	Joback Method
cpg	524.47	J/mol×K	855.78	Joback Method
cpg	513.41	J/mol×K	814.65	Joback Method

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R536119&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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