Clorazepate M (hydroxy-), isomer 1, hydrolysis, acetylated

Inchi: InChI=1S/C17H14ClNO4/c1-10(20)19-15-8-7-12(18)9-14(15)17(22)13-5-3-4-6-16(13)23-

InchiKey: CCCYGCUEGYDYMZ-UHFFFAOYSA-N

Formula: C17H14ClNO4

SMILES: CC(=O)Nc1ccc(Cl)cc1C(=O)c1ccccc1OC(C)=O

Mol. weight [g/mol]: 331.75

Physical Properties

Property code	Value	Unit	Source
gf	-126.11	kJ/mol	Joback Method
hf	-387.79	kJ/mol	Joback Method
hfus	41.98	kJ/mol	Joback Method
hvap	93.44	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.455		Crippen Method
mcvol	235.670	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	2560.00		NIST Webbook
rinpol	2560.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2560.00		NIST Webbook
tb	928.29	K	Joback Method
tc	1170.75	K	Joback Method
tf	626.35	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.39	J/mol×K	928.29	Joback Method
cpg	674.16	J/mol×K	968.70	Joback Method
cpg	682.76	J/mol×K	1009.11	Joback Method
cpg	690.22	J/mol×K	1049.52	Joback Method
cpg	696.60	J/mol×K	1089.93	Joback Method
cpg	701.93	J/mol×K	1130.34	Joback Method

cpg	706.25	J/mol×K	1170.75	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=R312913&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