Quazepam + M (oxo-), hydrolysis

Inchi: InChI=1S/C15H10ClF4NO/c16-9-5-6-13(21-8-15(18,19)20)11(7-9)14(22)10-3-1-2-4-12(1
InchiKey: VGNVFAXJHFXDAT-UHFFFAOYSA-N
Formula: C15H10ClF4NO
SMILES: O=C(c1ccccc1F)c1cc(Cl)ccc1NCC(F)(F)F
Mol. weight [g/mol]: 331.69

Physical Properties

Property code	Value	Unit	Source
gf	-556.51	kJ/mol	Joback Method
hf	-782.32	kJ/mol	Joback Method
hfus	37.32	kJ/mol	Joback Method
hvap	68.53	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.684		Crippen Method
mcvol	205.560	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1985.00		NIST Webbook
tb	746.22	K	Joback Method
tc	963.44	K	Joback Method
tf	486.50	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.76	J/mol×K	746.22	Joback Method
cpg	559.25	J/mol×K	782.42	Joback Method
cpg	569.79	J/mol×K	818.63	Joback Method
cpg	579.46	J/mol×K	854.83	Joback Method
cpg	588.34	J/mol×K	891.04	Joback Method
cpg	596.49	J/mol×K	927.24	Joback Method
cpg	603.98	J/mol×K	963.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313436&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

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