bis-desalkyl-metaclazepam

Inchi: InChI=1S/C16H14BrClN2O/c17-10-5-6-15-13(7-10)16(19-8-11(9-21)20-15)12-3-1-2-4-14
InchiKey: AMTVRNWGMLPECY-UHFFFAOYSA-N
Formula: C16H14BrClN2O
SMILES: OCC1CN=C(c2ccccc2Cl)c2cc(Br)ccc2N1
Mol. weight [g/mol]: 365.65

Physical Properties

Property code	Value	Unit	Source
gf	406.71	kJ/mol	Joback Method
hf	139.01	kJ/mol	Joback Method
hfus	47.18	kJ/mol	Joback Method
hvap	99.43	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.726		Crippen Method
mcvol	229.190	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	2850.00		NIST Webbook
tb	951.22	K	Joback Method
tc	1212.00	K	Joback Method
tf	711.77	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.93	J/mol×K	951.22	Joback Method
cpg	668.27	J/mol×K	994.68	Joback Method
cpg	677.30	J/mol×K	1038.15	Joback Method
cpg	685.10	J/mol×K	1081.61	Joback Method
cpg	691.73	J/mol×K	1125.07	Joback Method
cpg	697.26	J/mol×K	1168.53	Joback Method
cpg	701.75	J/mol×K	1212.00	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=R522284&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume