N-desmethyl-metaclazepam

Inchi: InChI=1S/C17H16BrClN2O/c1-22-10-12-9-20-17(13-4-2-3-5-15(13)19)14-8-11(18)6-7-16
InchiKey: KFWTVKIBHPHOPT-UHFFFAOYSA-N
Formula: C17H16BrClN2O
SMILES: COCC1CN=C(c2ccccc2Cl)c2cc(Br)ccc2N1
Mol. weight [g/mol]: 379.68
CAS: 86298-26-2

Physical Properties

Property code	Value	Unit	Source
gf	446.95	kJ/mol	Joback Method
hf	138.38	kJ/mol	Joback Method
hfus	46.87	kJ/mol	Joback Method
hvap	87.38	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.380		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	2690.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook
tb	904.34	K	Joback Method
tc	1178.26	K	Joback Method
tf	684.45	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.76	J/mol×K	904.34	Joback Method
cpg	708.18	J/mol×K	949.99	Joback Method
cpg	719.84	J/mol×K	995.65	Joback Method
cpg	729.77	J/mol×K	1041.30	Joback Method
cpg	738.02	J/mol×K	1086.95	Joback Method
cpg	744.63	J/mol×K	1132.61	Joback Method

cpg	749.66	J/mol×K	1178.26	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=C86298262&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