Diazepoxide M (nor-desoxo)

Inchi: InChI=1S/C15H12ClN3/c16-11-6-7-13-12(8-11)15(18-9-14(17)19-13)10-4-2-1-3-5-10/h1-
InchiKey: UMBZDAJGYNJMGS-UHFFFAOYSA-N
Formula: C15H12ClN3
SMILES: NC1=Nc2ccc(Cl)cc2C(c2ccccc2)=NC1
Mol. weight [g/mol]: 269.73

Physical Properties

Property code	Value	Unit	Source
gf	653.98	kJ/mol	Joback Method
hf	430.62	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	84.78	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.180		Crippen Method
mcvol	197.410	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	2452.00		NIST Webbook
tb	851.51	K	Joback Method
tc	1144.07	K	Joback Method
tf	634.65	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.30	J/mol×K	851.51	Joback Method
cpg	589.83	J/mol×K	900.27	Joback Method
cpg	601.42	J/mol×K	949.03	Joback Method
cpg	611.14	J/mol×K	997.79	Joback Method
cpg	619.06	J/mol×K	1046.55	Joback Method
cpg	625.24	J/mol×K	1095.31	Joback Method
cpg	629.75	J/mol×K	1144.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R311301&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