3H-1,4-Benzodiazepin-2-amine, 7-chloro-N-methyl-5-phenyl-

Other names: Chlordiazepam
Desoxychlordiazepoxide
RCDZ
3H-1,4-Benzodiazepine, 7-chloro-2-(methylamino)-5-phenyl-
Chlordiazepoxide M (desoxo)

Inchi: InChI=1S/C16H14ClN3/c1-18-15-10-19-16(11-5-3-2-4-6-11)13-9-12(17)7-8-14(13)20-15/

InchiKey: FAMNQSVPYUAUAF-UHFFFAOYSA-N

Formula: C16H14ClN3

SMILES: CNC1=Nc2ccc(Cl)cc2C(c2ccccc2)=NC1

Mol. weight [g/mol]: 283.75

CAS: 4393-72-0

Physical Properties

Property code	Value	Unit	Source
gf	685.34	kJ/mol	Joback Method
hf	429.66	kJ/mol	Joback Method
hfus	38.60	kJ/mol	Joback Method
hvap	82.80	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.440		Crippen Method
mcvol	211.500	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
rinpol	2516.00		NIST Webbook
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
rinpol	2520.00		NIST Webbook
rinpol	2516.00		NIST Webbook
rinpol	2500.00		NIST Webbook
tb	852.03	K	Joback Method
tc	1129.55	K	Joback Method
tf	615.32	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.78	J/mol×K	852.03	Joback Method
cpg	639.08	J/mol×K	898.28	Joback Method
cpg	651.51	J/mol×K	944.54	Joback Method
cpg	662.14	J/mol×K	990.79	Joback Method
cpg	671.03	J/mol×K	1037.05	Joback Method
cpg	678.24	J/mol×K	1083.30	Joback Method
cpg	683.84	J/mol×K	1129.55	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4393720&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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