7-Aminonorflunitrazepam

Other names: 7-Amino-desmethylflunitrazepam
Inchi: InChI=1S/C15H12FN3O/c16-12-4-2-1-3-10(12)15-11-7-9(17)5-6-13(11)19-14(20)8-18-15
InchiKey: IWZVUERQZJRRPL-UHFFFAOYSA-N
Formula: C15H12FN3O
SMILES: Nc1ccc2c(c1)C(c1ccccc1F)=NCC(=O)N2
Mol. weight [g/mol]: 269.27

Physical Properties

Property code	Value	Unit	Source
gf	289.48	kJ/mol	Joback Method
hf	21.61	kJ/mol	Joback Method
hfus	37.73	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.197		Crippen Method
mcvol	192.810	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	2825.00		NIST Webbook
rinpol	2825.00		NIST Webbook
tb	876.86	K	Joback Method
tc	1157.92	K	Joback Method
tf	706.27	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.52	J/mol×K	876.86	Joback Method
cpg	600.42	J/mol×K	923.70	Joback Method
cpg	611.42	J/mol×K	970.55	Joback Method
cpg	620.50	J/mol×K	1017.39	Joback Method
cpg	627.67	J/mol×K	1064.23	Joback Method
cpg	632.93	J/mol×K	1111.08	Joback Method
cpg	636.28	J/mol×K	1157.92	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=R17444&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