N-Desmethylflunitrazepam

Other names:	2H-1,4-Benzodiazepin-2-one, 5-(2-fluorophenyl)-1,3-dihydro-7-nitro-
	Flunitrazepan, N-desmethyl
	Norflunitrazepam
	Desmethylflunitrazepam
	5-(2-fluorophenyl)-1,3-dihydro-7-nitro-2H-1,4-benzodiazepin-2-one
Inchi:	InChI=1S/C15H10FN3O3/c16-12-4-2-1-3-10(12)15-11-7-9(19(21)22)5-6-13(11)18-14(20)
InchiKey:	KNGIGRDYBQPXKQ-UHFFFAOYSA-N
Formula:	C15H10FN3O3
SMILES:	O=C1CN=C(c2ccccc2F)c2cc([N+](=O)[O-])ccc2N1
Mol. weight [g/mol]:	299.26
CAS:	2558-30-7

Physical Properties

Property code	Value	Unit	Source
gf	258.58	kJ/mol	Joback Method
hf	-22.94	kJ/mol	Joback Method
hfus	43.90	kJ/mol	Joback Method
hvap	90.03	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.523		Crippen Method
mcvol	200.250	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2814.50		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2735.00		NIST Webbook
rinpol	2814.50		NIST Webbook
rinpol	2745.00		NIST Webbook
rinpol	2735.00		NIST Webbook
rinpol	2745.00		NIST Webbook
tb	956.17	K	Joback Method
tc	1247.68	K	Joback Method
tf	766.62	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.76	J/mol×K	956.17	Joback Method
cpg	628.47	J/mol×K	1004.75	Joback Method
cpg	636.08	J/mol×K	1053.34	Joback Method
cpg	641.60	J/mol×K	1101.92	Joback Method
cpg	645.04	J/mol×K	1150.51	Joback Method
cpg	646.41	J/mol×K	1199.09	Joback Method
cpg	645.70	J/mol×K	1247.68	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=C2558307&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