2,3-Dihydro-4-methyl-7-nitro-1H-1,5-benzodiazepi

Inchi: InChI=1S/C10H9N3O3/c1-6-4-10(14)12-8-3-2-7(13(15)16)5-9(8)11-6/h2-3,5H,4H2,1H3,(
InchiKey: XRCMCWYNHVSDJX-UHFFFAOYSA-N
Formula: C10H9N3O3
SMILES: CC1=Nc2cc([N+](=O)[O-])ccc2NC(=O)C1
Mol. weight [g/mol]: 219.20
CAS: 37546-86-4

Physical Properties

Property code	Value	Unit	Source
gf	308.51	kJ/mol	Joback Method
hf	51.31	kJ/mol	Joback Method
hfus	34.21	kJ/mol	Joback Method
hvap	76.78	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.029		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
tb	810.84	K	Joback Method
tc	1100.61	K	Joback Method
tf	670.74	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.74	J/mol×K	810.84	Joback Method
cpg	456.58	J/mol×K	859.14	Joback Method
cpg	467.71	J/mol×K	907.43	Joback Method
cpg	477.10	J/mol×K	955.73	Joback Method
cpg	484.72	J/mol×K	1004.02	Joback Method
cpg	490.51	J/mol×K	1052.32	Joback Method
cpg	494.46	J/mol×K	1100.61	Joback Method

Sources

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=C37546864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume