

9-Nitro triptycene

Inchi:	InChI=1S/C20H13NO2/c22-21(23)20-16-10-4-1-7-13(16)19(14-8-2-5-11-17(14)20)15-9-3
InchiKey:	ZCDJEBGVXDZZQH-UHFFFAOYSA-N
Formula:	C20H13NO2
SMILES:	O=[N+](O-)C12c3ccccc3C(c3ccccc31)c1ccccc12
Mol. weight [g/mol]:	299.32
CAS:	797-67-1

Physical Properties

Property code	Value	Unit	Source
gf	625.82	kJ/mol	Joback Method
hf	393.77	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	83.51	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	4.062		Crippen Method
mcvol	217.080	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	900.46	K	Joback Method
tc	1184.71	K	Joback Method
tf	649.45	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.03	J/molxK	900.46	Joback Method
cpg	671.09	J/molxK	947.84	Joback Method
cpg	690.34	J/molxK	995.21	Joback Method
cpg	711.33	J/molxK	1042.59	Joback Method
cpg	734.61	J/molxK	1089.96	Joback Method
cpg	760.73	J/molxK	1137.34	Joback Method
cpg	790.25	J/molxK	1184.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C797671&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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