4-NITRO-2-(TRIFLUOROMETHYL)ANILINE

Other names: 4-Nitro-a,a,a-trifluoro-o-toluidine
Benzenamine, 4-nitro-2-(trifluoromethyl)-
4-nitro-«alpha»,«alpha»,«alpha»-trifluoro-o-toluidine
Inchi: InChI=1S/C7H5F3N2O2/c8-7(9,10)5-3-4(12(13)14)1-2-6(5)11/h1-3H,11H2
InchiKey: HOTZLWVITTVZGY-UHFFFAOYSA-N
Formula: C7H5F3N2O2
SMILES: Nc1ccc([N+](=O)[O-])cc1C(F)(F)F
Mol. weight [g/mol]: 206.12

Physical Properties

Property code	Value	Unit	Source
hf	-584.86	kJ/mol	Cheméo Relay (1.0)
hfus	25.53	kJ/mol	Joback Method
hvap	71.06	kJ/mol	Cheméo Relay (1.0)
ie	9.01	eV	Cheméo Relay (1.0)
log10ws	-3.05		Cheméo Relay (1.0)
logp	2.196		Crippen Method
mcvol	118.440	ml/mol	McGowan Method
tb	529.87	K	Cheméo Relay (1.0)
tf	359.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.10	J/mol×K	615.15	Joback Method
cpg	307.46	J/mol×K	654.52	Joback Method
cpg	315.99	J/mol×K	693.88	Joback Method
cpg	323.75	J/mol×K	733.25	Joback Method
cpg	330.80	J/mol×K	772.62	Joback Method
cpg	337.20	J/mol×K	811.98	Joback Method
cpg	343.01	J/mol×K	851.35	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C121017&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point