o-Cresol, 6-nitro-

Other names: o-Cresol, 6-nitro-,
Inchi: InChI=1S/C7H7NO3/c1-5-3-2-4-6(7(5)9)8(10)11/h2-4,9H,1H3
InchiKey: AQDKZPFDOWHRDZ-UHFFFAOYSA-N
Formula: C7H7NO3
SMILES: Cc1cccc([N+](=O)[O-])c1O
Mol. weight [g/mol]: 153.14

Physical Properties

Property code	Value	Unit	Source
hf	-142.87	kJ/mol	Cheméo Relay (1.0)
hfus	24.68	kJ/mol	Joback Method
hvap	68.12	kJ/mol	Cheméo Relay (1.0)
ie	8.79	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	1.609		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
rinpol	1270.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1305.00		NIST Webbook
tb	519.05	K	Cheméo Relay (1.0)
tc	792.95	K	Cheméo Relay (1.0)
tf	326.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.28	J/mol×K	623.68	Joback Method
cpg	271.81	J/mol×K	667.01	Joback Method
cpg	280.56	J/mol×K	710.34	Joback Method
cpg	288.66	J/mol×K	753.67	Joback Method
cpg	296.21	J/mol×K	797.01	Joback Method
cpg	303.32	J/mol×K	840.34	Joback Method
cpg	310.10	J/mol×K	883.67	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13073295&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point