2-BROMOMETHYL-4-NITROPHENOL

Other names: «alpha»-Bromo-4-nitro-o-cresol
Phenol, 2-(bromomethyl)-4-nitro-
o-Cresol, «alpha»-bromo-4-nitro-
Alpha-bromo-4-nitro-O-cresol
Inchi: InChI=1S/C7H6BrNO3/c8-4-5-3-6(9(11)12)1-2-7(5)10/h1-3,10H,4H2
InchiKey: KFDPCYZHENQOBV-UHFFFAOYSA-N
Formula: C7H6BrNO3
SMILES: O=[N+]([O-])c1ccc(O)c(CBr)c1
Mol. weight [g/mol]: 232.03

Physical Properties

Property code	Value	Unit	Source
hf	-121.83	kJ/mol	Cheméo Relay (1.0)
hfus	29.97	kJ/mol	Joback Method
hvap	89.32	kJ/mol	Cheméo Relay (1.0)
ie	9.20	eV	Cheméo Relay (1.0)
log10ws	-2.66		Cheméo Relay (1.0)
logp	2.195		Crippen Method
mcvol	126.520	ml/mol	McGowan Method
tb	574.41	K	Cheméo Relay (1.0)
tf	414.06	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.25	J/mol×K	689.84	Joback Method
cpg	296.48	J/mol×K	735.10	Joback Method
cpg	304.08	J/mol×K	780.37	Joback Method
cpg	311.18	J/mol×K	825.63	Joback Method
cpg	317.94	J/mol×K	870.90	Joback Method
cpg	324.51	J/mol×K	916.16	Joback Method
cpg	331.01	J/mol×K	961.43	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C772338&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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point