6-BROMOHEXANENITRILE

Other names:	5-Bromopentyl cyanide
	6-Bromocapronitrile
	6-Bromohexanonitrile
	Hexanenitrile, 6-bromo-
Inchi:	InChI=1S/C6H10BrN/c7-5-3-1-2-4-6-8/h1-5H2
InchiKey:	PHOSWLARCIBBJZ-UHFFFAOYSA-N
Formula:	C6H10BrN
SMILES:	N#CCCCCCBr
Mol. weight [g/mol]:	176.06

Physical Properties

Property code	Value	Unit	Source
af	0.5723		Cheméo Relay (1.0)
hf	9.02	kJ/mol	Cheméo Relay (1.0)
hfus	18.09	kJ/mol	Joback Method
hvap	63.35	kJ/mol	Cheméo Relay (1.0)
ie	10.86	eV	Cheméo Relay (1.0)
logp	2.465		Crippen Method
mcvol	114.280	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	511.40	K	Cheméo Relay (1.0)
tc	707.42	K	Cheméo Relay (1.0)
tf	264.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.60	J/mol×K	504.92	Joback Method
cpg	231.51	J/mol×K	539.11	Joback Method
cpg	239.95	J/mol×K	573.29	Joback Method
cpg	247.94	J/mol×K	607.48	Joback Method
cpg	255.51	J/mol×K	641.67	Joback Method
cpg	262.67	J/mol×K	675.85	Joback Method
cpg	269.45	J/mol×K	710.04	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6621596&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
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