2-(p-Chlorophenyl)-3-methylbutyronitrile

Other names: Benzeneacetonitrile, 4-chloro-«alpha»-(1-methylethyl)-
2-(4-chlorophenyl)-3-methylbutyronitrile
Inchi: InChI=1S/C11H12ClN/c1-8(2)11(7-13)9-3-5-10(12)6-4-9/h3-6,8,11H,1-2H3
InchiKey: RBGSZIRWNWQDOK-UHFFFAOYSA-N
Formula: C11H12ClN
SMILES: CC(C)C(C#N)c1ccc(Cl)cc1
Mol. weight [g/mol]: 193.67
CAS: 2012-81-9

Physical Properties

Property code	Value	Unit	Source
gf	260.89	kJ/mol	Joback Method
hf	93.27	kJ/mol	Joback Method
hfus	16.56	kJ/mol	Joback Method
hvap	57.11	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.603		Crippen Method
mcvol	155.710	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
tb	621.37	K	Joback Method
tc	854.93	K	Joback Method
tf	317.58	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.45	J/mol×K	621.37	Joback Method
cpg	372.26	J/mol×K	660.30	Joback Method
cpg	384.18	J/mol×K	699.22	Joback Method
cpg	395.26	J/mol×K	738.15	Joback Method
cpg	405.53	J/mol×K	777.08	Joback Method
cpg	415.05	J/mol×K	816.01	Joback Method
cpg	423.85	J/mol×K	854.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.50 ± 1.50	K	0.01	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2012819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume