1-Chloromethyl-4-methylnaphthalene

Inchi: InChI=1S/C12H11Cl/c1-9-6-7-10(8-13)12-5-3-2-4-11(9)12/h2-7H,8H2,1H3
InchiKey: QHXSBKTZBDHBKF-UHFFFAOYSA-N
Formula: C12H11Cl
SMILES: Cc1ccc(CCl)c2ccccc12
Mol. weight [g/mol]: 190.67
CAS: 5261-50-7

Physical Properties

Property code	Value	Unit	Source
gf	238.03	kJ/mol	Joback Method
hf	97.91	kJ/mol	Joback Method
hfus	21.32	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.887		Crippen Method
mcvol	148.960	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	567.01	K	Joback Method
tc	802.92	K	Joback Method
tf	339.08	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.55	J/mol×K	567.01	Joback Method
cpg	382.30	J/mol×K	763.60	Joback Method
cpg	372.06	J/mol×K	724.28	Joback Method
cpg	361.04	J/mol×K	684.97	Joback Method
cpg	349.17	J/mol×K	645.65	Joback Method
cpg	336.36	J/mol×K	606.33	Joback Method
cpg	391.82	J/mol×K	802.92	Joback Method

dvisc	0.0003186	Pa×s	567.01	Joback Method
dvisc	0.0003730	Pa×s	529.02	Joback Method
dvisc	0.0004475	Pa×s	491.03	Joback Method
dvisc	0.0005535	Pa×s	453.05	Joback Method
dvisc	0.0007117	Pa×s	415.06	Joback Method
dvisc	0.0009629	Pa×s	377.07	Joback Method
dvisc	0.0013939	Pa×s	339.08	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5261507&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume