1-CHLOROMETHYL-3-(1,1-DIMETHYLETHYL)BEN

Other names: Benzene,1-(chloromethyl)-3-dimethylethyl)-
Inchi: InChI=1S/C11H15Cl/c1-11(2,3)10-6-4-5-9(7-10)8-12/h4-7H,8H2,1-3H3
InchiKey: QZWCABOLGIVZCP-UHFFFAOYSA-N
Formula: C11H15Cl
SMILES: CC(C)(C)c1cccc(CCl)c1
Mol. weight [g/mol]: 182.69

Physical Properties

Property code	Value	Unit	Source
af	0.3785		Cheméo Relay (1.0)
hf	-107.65	kJ/mol	Cheméo Relay (1.0)
hfus	14.68	kJ/mol	Joback Method
hvap	59.70	kJ/mol	Cheméo Relay (1.0)
ie	8.71 ± 0.03	eV	NIST Webbook
log10ws	-4.64		Cheméo Relay (1.0)
logp	3.723		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
tb	511.19	K	Cheméo Relay (1.0)
tc	731.47	K	Cheméo Relay (1.0)
tf	290.11	K	Cheméo Relay (1.0)
vc	0.551	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.36	J/mol×K	516.94	Joback Method
cpg	349.41	J/mol×K	553.98	Joback Method
cpg	364.38	J/mol×K	591.01	Joback Method
cpg	378.31	J/mol×K	628.05	Joback Method
cpg	391.28	J/mol×K	665.09	Joback Method
cpg	403.35	J/mol×K	702.12	Joback Method
cpg	414.58	J/mol×K	739.16	Joback Method
dvisc	0.0032297	Pa×s	285.01	Joback Method

dvisc	0.0015576	Pa×s	323.67	Joback Method
dvisc	0.0008777	Pa×s	362.32	Joback Method
dvisc	0.0005524	Pa×s	400.98	Joback Method
dvisc	0.0003772	Pa×s	439.63	Joback Method
dvisc	0.0002739	Pa×s	478.29	Joback Method
dvisc	0.0002087	Pa×s	516.94	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C38580799&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):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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