1,3,5-Trimethyl-1-cyclohexene,c&t

Other names: Cyclohexene, 1,3,5-trimethyl-
1,3,5-Trimethyl-1-cyclohexene,c&t
Inchi: InChI=1S/C9H16/c1-7-4-8(2)6-9(3)5-7/h4,7,9H,5-6H2,1-3H3
InchiKey: PKHOIUJRGGWFEF-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC1=CC(C)CC(C)C1
Mol. weight [g/mol]: 124.22
CAS: 3643-64-9

Physical Properties

Property code	Value	Unit	Source
gf	61.97	kJ/mol	Joback Method
hf	-148.80	kJ/mol	Joback Method
hfus	12.80	kJ/mol	Joback Method
hvap	36.70	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.999		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	414.40 ± 3.00	K	NIST Webbook
tb	413.00 ± 3.00	K	NIST Webbook
tb	414.20	K	NIST Webbook
tc	626.38	K	Joback Method
tf	207.61	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.33	J/mol×K	424.34	Joback Method
cpg	260.46	J/mol×K	458.01	Joback Method
cpg	276.84	J/mol×K	491.69	Joback Method
cpg	292.47	J/mol×K	525.36	Joback Method
cpg	307.37	J/mol×K	559.03	Joback Method

cpg	321.55	J/mol×K	592.70	Joback Method
cpg	335.03	J/mol×K	626.38	Joback Method
dvisc	0.0021413	Pa×s	207.61	Joback Method
dvisc	0.0011365	Pa×s	243.73	Joback Method
dvisc	0.0007103	Pa×s	279.85	Joback Method
dvisc	0.0004943	Pa×s	315.98	Joback Method
dvisc	0.0003706	Pa×s	352.10	Joback Method
dvisc	0.0002931	Pa×s	388.22	Joback Method
dvisc	0.0002413	Pa×s	424.34	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3643649&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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