Methylcyclododecane

Other names: Cyclododecane, methyl
Inchi: InChI=1S/C13H26/c1-13-11-9-7-5-3-2-4-6-8-10-12-13/h13H,2-12H2,1H3
InchiKey: MAJAJAXSPRXRRS-UHFFFAOYSA-N
Formula: C13H26
SMILES: CC1CCCCCCCCCCC1
Mol. weight [g/mol]: 182.35

Physical Properties

Property code	Value	Unit	Source
gf	10.43	kJ/mol	Joback Method
hf	-294.29	kJ/mol	Joback Method
hfus	8.66	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.927		Crippen Method
mcvol	183.170	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1379.00		NIST Webbook
tb	542.01	K	Joback Method
tc	777.69	K	Joback Method
tf	222.53	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.19	J/mol×K	542.01	Joback Method
cpg	482.96	J/mol×K	581.29	Joback Method
cpg	510.09	J/mol×K	620.57	Joback Method
cpg	535.57	J/mol×K	659.85	Joback Method
cpg	559.39	J/mol×K	699.13	Joback Method
cpg	581.54	J/mol×K	738.41	Joback Method
cpg	602.01	J/mol×K	777.69	Joback Method

dvisc	0.1307048	Pa×s	222.53	Joback Method
dvisc	0.0102052	Pa×s	275.78	Joback Method
dvisc	0.0018189	Pa×s	329.02	Joback Method
dvisc	0.0005241	Pa×s	382.27	Joback Method
dvisc	0.0002047	Pa×s	435.52	Joback Method
dvisc	0.0000982	Pa×s	488.76	Joback Method
dvisc	0.0000544	Pa×s	542.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R2618&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

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