(E,E,E)-1,5,9-Cyclododecatriene, 3-methyl

Inchi: InChI=1S/C13H20/c1-13-11-9-7-5-3-2-4-6-8-10-12-13/h2-3,8-11,13H,4-7,12H2,1H3/b3-2
InchiKey: OQDOPRBIIHXPJP-PVXCSLJCSA-N
Formula: C13H20
SMILES: CC1C=CCCC=CCCC=CC1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	100.31	kJ/mol	Joback Method
hf	-120.95	kJ/mol	Joback Method
hfus	12.33	kJ/mol	Joback Method
hvap	46.87	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.255		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1308.00		NIST Webbook
tb	539.49	K	Joback Method
tc	782.60	K	Joback Method
tf	224.81	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.08	J/mol×K	539.49	Joback Method
cpg	423.24	J/mol×K	580.01	Joback Method
cpg	446.86	J/mol×K	620.53	Joback Method
cpg	468.92	J/mol×K	661.04	Joback Method
cpg	489.42	J/mol×K	701.56	Joback Method
cpg	508.36	J/mol×K	742.08	Joback Method
cpg	525.73	J/mol×K	782.60	Joback Method
dvisc	0.0547834	Pa×s	224.81	Joback Method
dvisc	0.0058834	Pa×s	277.26	Joback Method

dvisc	0.0012850	Pa×s	329.70	Joback Method
dvisc	0.0004261	Pa×s	382.15	Joback Method
dvisc	0.0001844	Pa×s	434.60	Joback Method
dvisc	0.0000956	Pa×s	487.04	Joback Method
dvisc	0.0000563	Pa×s	539.49	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=R2765&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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