3-Cedrene

Inchi: InChI=1S/C15H24/c1-10-7-8-15-9-12(10)14(3,4)13(15)6-5-11(15)2/h5-6,10-13H,7-9H2,1-
InchiKey: FLNQYYHEHVZOFX-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1CCC23CC1C(C)(C)C2C=CC3C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	229.32	kJ/mol	Joback Method
hf	-119.61	kJ/mol	Joback Method
hfus	16.65	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1398.00		NIST Webbook
tb	556.99	K	Joback Method
tc	781.41	K	Joback Method
tf	341.43	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.19	J/mol×K	556.99	Joback Method
cpg	527.15	J/mol×K	594.39	Joback Method
cpg	549.41	J/mol×K	631.80	Joback Method
cpg	570.27	J/mol×K	669.20	Joback Method
cpg	590.02	J/mol×K	706.60	Joback Method
cpg	608.95	J/mol×K	744.01	Joback Method
cpg	627.34	J/mol×K	781.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190639&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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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