«alpha»-Cyperene

Inchi: InChI=1S/C15H24/c1-10-7-8-15-11(2)5-6-12(9-13(10)15)14(15,3)4/h11-12H,5-9H2,1-4H3
InchiKey: RTBLDXVIGWSICW-JMSVASOKSA-N
Formula: C15H24
SMILES: CC1=C2CC3CCC(C)C2(CC1)C3(C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	225.48	kJ/mol	Joback Method
hf	-101.87	kJ/mol	Joback Method
hfus	13.73	kJ/mol	Joback Method
hvap	48.07	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1350.00		NIST Webbook
tb	576.29	K	Joback Method
tc	802.89	K	Joback Method
tf	374.95	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.46	J/mol×K	576.29	Joback Method
cpg	525.54	J/mol×K	614.06	Joback Method
cpg	546.15	J/mol×K	651.82	Joback Method
cpg	565.60	J/mol×K	689.59	Joback Method
cpg	584.18	J/mol×K	727.36	Joback Method
cpg	602.19	J/mol×K	765.12	Joback Method
cpg	619.93	J/mol×K	802.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R432765&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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