cycloeucalane

Inchi: InChI=1S/C30H52/c1-20(2)21(3)10-11-23(5)24-14-16-28(7)26-13-12-25-22(4)9-8-15-29(
InchiKey: GYQYLPXFYDCSFX-YPOKRKHXSA-N
Formula: C30H52
SMILES: CC(C)C(C)CCC(C)C1CCC2(C)C3CCC4C(C)CCCC45CC35CCC12C
Mol. weight [g/mol]: 412.73
CAS: 469-40-9

Physical Properties

Property code	Value	Unit	Source
gf	416.76	kJ/mol	Joback Method
hf	-332.91	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	75.76	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	9.134		Crippen Method
mcvol	379.260	ml/mol	McGowan Method
pc	936.35	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3040.00		NIST Webbook
rinpol	3092.00		NIST Webbook
tb	917.94	K	Joback Method
tc	1148.01	K	Joback Method
tf	544.88	K	Joback Method
vc	1.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1431.63	J/mol×K	917.94	Joback Method
cpg	1472.52	J/mol×K	956.28	Joback Method
cpg	1515.72	J/mol×K	994.63	Joback Method
cpg	1561.87	J/mol×K	1032.97	Joback Method
cpg	1611.60	J/mol×K	1071.32	Joback Method
cpg	1665.52	J/mol×K	1109.66	Joback Method

cpg	1724.28	J/mol×K	1148.01	Joback Method

Sources

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=C469409&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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