Modhephene

Other names: Modheph-2-ene
Inchi: InChI=1S/C15H24/c1-11-6-9-14-7-5-8-15(11,14)12(2)10-13(14,3)4/h10-11H,5-9H2,1-4H3
InchiKey: APGXRXFCBZKIAN-JBAPVGOWSA-N
Formula: C15H24
SMILES: CC1=CC(C)(C)C23CCCC12C(C)CC3
Mol. weight [g/mol]: 204.35
CAS: 68269-87-4

Physical Properties

Property code	Value	Unit	Source
gf	229.62	kJ/mol	Joback Method
hf	-75.16	kJ/mol	Joback Method
hfus	7.82	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1385.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1392.30		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1385.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1499.00		NIST Webbook
ripol	1522.00		NIST Webbook
ripol	1522.00		NIST Webbook

ripol	1496.00		NIST Webbook
tb	571.55	K	Joback Method
tc	806.48	K	Joback Method
tf	386.33	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.53	J/mol×K	571.55	Joback Method
cpg	523.86	J/mol×K	610.71	Joback Method
cpg	544.56	J/mol×K	649.86	Joback Method
cpg	564.09	J/mol×K	689.02	Joback Method
cpg	582.88	J/mol×K	728.17	Joback Method
cpg	601.40	J/mol×K	767.33	Joback Method
cpg	620.08	J/mol×K	806.48	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C68269874&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume