Modhephene

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-BYCMXARLSA-N
Formula: C15H24
SMILES: CC1=CC(C)(C)C23CCCC12C(C)CC3
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
hfus	7.82	kJ/mol	Joback Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
rinpol	1385.00		NIST Webbook

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=R604292&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices