1,3-Dimethyl-5-ethyladamantane

Other names:	5-Ethyl-1,3-dimethyladamantane
	1-Ethyl-3,5-dimethyladamantane
	1-ethyl-3,5-methyladamantane
Inchi:	InChI=1S/C14H24/c1-4-14-7-11-5-12(2,9-14)8-13(3,6-11)10-14/h11H,4-10H2,1-3H3
InchiKey:	FTNPDAKMYKMVKB-UHFFFAOYSA-N
Formula:	C14H24
SMILES:	CCC12CC3CC(C)(CC(C)(C3)C1)C2
Mol. weight [g/mol]:	192.34
CAS:	1687-35-0

Physical Properties

Property code	Value	Unit	Source
gf	212.97	kJ/mol	Joback Method
hf	-94.67	kJ/mol	Joback Method
hfus	6.50	kJ/mol	Joback Method
hvap	42.91	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.393		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1313.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1321.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1303.00		NIST Webbook

rinpol	1287.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1406.00		NIST Webbook
tb	540.26	K	Joback Method
tc	767.88	K	Joback Method
tf	365.30	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.57	J/mol×K	540.26	Joback Method
cpg	490.29	J/mol×K	578.20	Joback Method
cpg	511.11	J/mol×K	616.13	Joback Method
cpg	530.47	J/mol×K	654.07	Joback Method
cpg	548.77	J/mol×K	692.01	Joback Method
cpg	566.45	J/mol×K	729.94	Joback Method
cpg	583.92	J/mol×K	767.88	Joback Method

Sources

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=C1687350&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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