1-n-butyladamantane

Other names: 1-Butyladamantane
Inchi: InChI=1S/C14H24/c1-2-3-4-14-8-11-5-12(9-14)7-13(6-11)10-14/h11-13H,2-10H2,1H3
InchiKey: AZCUIXHZJHFUFI-UHFFFAOYSA-N
Formula: C14H24
SMILES: CCCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 192.34
CAS: 14449-41-3

Physical Properties

Property code	Value	Unit	Source
gf	223.95	kJ/mol	Joback Method
hf	-125.15	kJ/mol	Joback Method
hfus	19.09	kJ/mol	Joback Method
hvap	45.21	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.393		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1479.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1443.00		NIST Webbook
tb	539.78	K	Joback Method
tc	749.54	K	Joback Method
tf	317.50	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.73	J/mol×K	539.78	Joback Method
cpg	491.44	J/mol×K	574.74	Joback Method
cpg	512.60	J/mol×K	609.70	Joback Method
cpg	532.39	J/mol×K	644.66	Joback Method
cpg	550.99	J/mol×K	679.62	Joback Method

cpg	568.57	J/mol×K	714.58	Joback Method
cpg	585.31	J/mol×K	749.54	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=C14449413&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume