

Anthracene, 9-butyltetradecahydro-

Other names:	9-n-Butyl-(tetradecahydroanthracene) 9-Butyltetradecahydroanthracene
Inchi:	InChI=1S/C18H32/c1-2-3-10-18-16-11-6-4-8-14(16)13-15-9-5-7-12-17(15)18/h14-18H,2-
InchiKey:	PJCBPPKQWYVHKO-UHFFFAOYSA-N
Formula:	C18H32
SMILES:	CCCCC1C2CCCCC2CC2CCCCC21
Mol. weight [g/mol]:	248.45
CAS:	55133-89-6

Physical Properties

Property code	Value	Unit	Source
gf	207.01	kJ/mol	Joback Method
hf	-267.93	kJ/mol	Joback Method
hfus	28.42	kJ/mol	Joback Method
hvap	55.64	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.809		Crippen Method
mvol	231.900	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
tb	643.47	K	Joback Method
tc	859.29	K	Joback Method
tf	320.36	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.60	J/molxK	643.47	Joback Method
cpg	730.24	J/molxK	679.44	Joback Method
cpg	756.14	J/molxK	715.41	Joback Method
cpg	780.39	J/molxK	751.38	Joback Method
cpg	803.06	J/molxK	787.35	Joback Method
cpg	824.25	J/molxK	823.32	Joback Method
cpg	844.02	J/molxK	859.29	Joback Method

dvisc	0.0032899	Paxs	320.36	Joback Method
dvisc	0.0020720	Paxs	374.21	Joback Method
dvisc	0.0014659	Paxs	428.06	Joback Method
dvisc	0.0011205	Paxs	481.92	Joback Method
dvisc	0.0009040	Paxs	535.77	Joback Method
dvisc	0.0007586	Paxs	589.62	Joback Method
dvisc	0.0006555	Paxs	643.47	Joback Method
hvapt	72.80	kJ/mol	438.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55133896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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