

5-Butyl-5-ethylpentadecane

Inchi:	InChI=1S/C21H44/c1-5-9-12-13-14-15-16-17-20-21(8-4,18-10-6-2)19-11-7-3/h5-20H2,1-4
InchiKey:	SXGMTXVWVIXGFE-UHFFFAOYSA-N
Formula:	C21H44
SMILES:	CCCCCCCCCCC(CC)(CCCC)CCCC
Mol. weight [g/mol]:	296.57

Physical Properties

Property code	Value	Unit	Source
gf	128.78	kJ/mol	Joback Method
hf	-485.52	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	61.04	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	8.294		Crippen Method
mcvol	306.750	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	1944.00		NIST Webbook
tb	676.65	K	Joback Method
tc	842.53	K	Joback Method
tf	328.85	K	Joback Method
vc	1.200	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.40	J/molxK	676.65	Joback Method
cpg	924.16	J/molxK	704.30	Joback Method
cpg	944.95	J/molxK	731.94	Joback Method
cpg	964.81	J/molxK	759.59	Joback Method
cpg	983.77	J/molxK	787.24	Joback Method
cpg	1001.89	J/molxK	814.88	Joback Method
cpg	1019.20	J/molxK	842.53	Joback Method
dvisc	0.0037943	Paxs	328.85	Joback Method
dvisc	0.0011988	Paxs	386.82	Joback Method

dvisc	0.0005115	Paxs	444.78	Joback Method
dvisc	0.0002656	Paxs	502.75	Joback Method
dvisc	0.0001579	Paxs	560.72	Joback Method
dvisc	0.0001035	Paxs	618.68	Joback Method
dvisc	0.0000729	Paxs	676.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360428&Units=SI

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
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

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