

11-Hexadecyn-1-ol

Inchi:	InChI=1S/C16H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h17H,2-4,7-16H2,1H3
InchiKey:	CWJKFTYJCIEEDB-UHFFFAOYSA-N
Formula:	C16H30O
SMILES:	CCCCC#CCCCCCCCCCCCO
Mol. weight [g/mol]:	238.41
CAS:	65686-49-9

Physical Properties

Property code	Value	Unit	Source
gf	149.82	kJ/mol	Joback Method
hf	-253.50	kJ/mol	Joback Method
hfus	44.41	kJ/mol	Joback Method
hvap	70.04	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.683		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
tb	666.66	K	Joback Method
tc	837.62	K	Joback Method
tf	437.00	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.81	J/mol×K	666.66	Joback Method
cpg	667.14	J/mol×K	695.15	Joback Method
cpg	682.75	J/mol×K	723.65	Joback Method
cpg	697.69	J/mol×K	752.14	Joback Method
cpg	711.97	J/mol×K	780.63	Joback Method
cpg	725.61	J/mol×K	809.13	Joback Method
cpg	738.63	J/mol×K	837.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65686499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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