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#CCCCCCCCCCO
Mol. weight [g/mol]: 238.42

Physical Properties

Property code	Value	Unit	Source
af	0.8718		Cheméo Relay (1.0)
gf	149.82	kJ/mol	Joback Method
hf	-276.67	kJ/mol	Cheméo Relay (1.0)
hfus	44.41	kJ/mol	Joback Method
hvap	104.93	kJ/mol	Cheméo Relay (1.0)
ie	9.45	eV	Cheméo Relay (1.0)
log10ws	-5.18		Cheméo Relay (1.0)
logp	4.683		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
tb	581.01	K	Cheméo Relay (1.0)
tc	777.16	K	Cheméo Relay (1.0)
tf	307.62	K	Cheméo Relay (1.0)
vc	0.874	m3/kmol	Cheméo Relay (1.0)

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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