

1-Heptacosanol

Other names:	Heptacosan-1-ol Heptacosanol
Inchi:	InChI=1S/C27H56O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-
InchiKey:	ULCZGKYHRYJXAU-UHFFFAOYSA-N
Formula:	C27H56O
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	396.73
CAS:	2004-39-9

Physical Properties

Property code	Value	Unit	Source
gf	39.64	kJ/mol	Joback Method
hf	-752.84	kJ/mol	Joback Method
hfus	69.77	kJ/mol	Joback Method
hvap	92.37	kJ/mol	Joback Method
log10ws	-10.39		Crippen Method
logp	9.751		Crippen Method
mcvol	397.160	ml/mol	McGowan Method
pc	723.40	kPa	Joback Method
rinpol	3016.00		NIST Webbook
rinpol	432.80		NIST Webbook
tb	909.34	K	Joback Method
tc	1126.29	K	Joback Method
tf	454.87	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1371.02	J/mol×K	909.34	Joback Method
cpg	1396.03	J/mol×K	945.50	Joback Method
cpg	1419.56	J/mol×K	981.66	Joback Method
cpg	1441.69	J/mol×K	1017.81	Joback Method
cpg	1462.52	J/mol×K	1053.97	Joback Method

cpg	1482.14	J/mol×K	1090.13	Joback Method
cpg	1500.63	J/mol×K	1126.29	Joback Method
dvisc	0.0008114	Pa×s	454.87	Joback Method
dvisc	0.0001932	Pa×s	530.62	Joback Method
dvisc	0.0000659	Pa×s	606.36	Joback Method
dvisc	0.0000285	Pa×s	682.11	Joback Method
dvisc	0.0000146	Pa×s	757.85	Joback Method
dvisc	0.0000084	Pa×s	833.60	Joback Method
dvisc	0.0000053	Pa×s	909.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44305e+01
Coeff. B	-5.78046e+03
Coeff. C	-1.34402e+02
Temperature range (K), min.	543.12
Temperature range (K), max.	768.29

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2004399&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
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
pvap:	Vapor 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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