

1-Octacosene

Other names:	Octacosene octacos-1-ene
Inchi:	InChI=1S/C28H56/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-28-26-24-22-20-18-16-14-12-10-8-6-4-2
InchiKey:	QEXZDYLACYKGOM-UHFFFAOYSA-N
Formula:	C28H56
SMILES:	C=CCCCCCCCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	392.74
CAS:	18835-34-2

Physical Properties

Property code	Value	Unit	Source
gf	272.72	kJ/mol	Joback Method
hf	-495.82	kJ/mol	Joback Method
hfus	67.00	kJ/mol	Joback Method
hvap	77.25	kJ/mol	Joback Method
log10ws	-11.40		Crippen Method
logp	10.945		Crippen Method
mcvol	401.080	ml/mol	McGowan Method
pc	669.77	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
rinpol	2794.00		NIST Webbook
tb	836.72	K	Joback Method
tc	1025.39	K	Joback Method
tf	403.56	K	Joback Method
vc	1.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1450.72	J/mol×K	1025.39	Joback Method
cpg	1431.61	J/mol×K	993.94	Joback Method
cpg	1411.48	J/mol×K	962.50	Joback Method
cpg	1390.29	J/mol×K	931.05	Joback Method

cpg	1367.96	J/mol×K	899.61	Joback Method
cpg	1344.43	J/mol×K	868.16	Joback Method
cpg	1319.64	J/mol×K	836.72	Joback Method
dvisc	0.0014117	Pa×s	403.56	Joback Method
dvisc	0.0000350	Pa×s	836.72	Joback Method
dvisc	0.0000485	Pa×s	764.53	Joback Method
dvisc	0.0000718	Pa×s	692.33	Joback Method
dvisc	0.0001166	Pa×s	620.14	Joback Method
dvisc	0.0002151	Pa×s	547.95	Joback Method
dvisc	0.0004777	Pa×s	475.75	Joback Method
hvapt	111.00	kJ/mol	575.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.20567e+01
Coeff. B	-3.37453e+03
Coeff. C	-2.46872e+02
Temperature range (K), min.	533.60
Temperature range (K), max.	747.16

Sources

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=C18835342&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

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
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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