

Octacosanoic acid

Other names:	Montanic acid Octacosanoic acid,synthetic
Inchi:	InChI=1S/C28H56O2/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:	UTOPWMOLSKOLTQ-UHFFFAOYSA-N
Formula:	C28H56O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	424.74
CAS:	506-48-9

Physical Properties

Property code	Value	Unit	Source
gf	-80.86	kJ/mol	Joback Method
hf	-886.06	kJ/mol	Joback Method
hfus	73.96	kJ/mol	Joback Method
hvap	101.35	kJ/mol	Joback Method
log10ws	-10.64		Crippen Method
logp	10.234		Crippen Method
mvol	412.820	ml/mol	McGowan Method
pc	710.73	kPa	Joback Method
tb	986.09	K	Joback Method
tc	1234.84	K	Joback Method
tf	516.07	K	Joback Method
vc	1.629	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.89	J/molxK	986.09	Joback Method
cpg	1488.13	J/molxK	1027.55	Joback Method
cpg	1511.59	J/molxK	1069.01	Joback Method
cpg	1533.41	J/molxK	1110.47	Joback Method
cpg	1553.74	J/molxK	1151.93	Joback Method
cpg	1572.71	J/molxK	1193.39	Joback Method
cpg	1590.45	J/molxK	1234.84	Joback Method

dvisc	0.0003594	Paxs	516.07	Joback Method
dvisc	0.0001025	Paxs	594.41	Joback Method
dvisc	0.0000392	Paxs	672.74	Joback Method
dvisc	0.0000183	Paxs	751.08	Joback Method
dvisc	0.0000099	Paxs	829.42	Joback Method
dvisc	0.0000059	Paxs	907.75	Joback Method
dvisc	0.0000038	Paxs	986.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.52624e+01
Coeff. B	-1.17645e+04
Coeff. C	-1.70264e+02
Temperature range (K), min.	641.32
Temperature range (K), max.	759.94

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C506489&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

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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