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: CCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 424.75
CAS: 506-48-9

Physical Properties

Property code	Value	Unit	Source
af	1.4598		Cheméo Relay (1.0)
gf	-80.86	kJ/mol	Joback Method
hf	-980.06	kJ/mol	Cheméo Relay (1.0)
hfus	73.96	kJ/mol	Joback Method
hvap	170.47	kJ/mol	Cheméo Relay (1.0)
ie	10.36	eV	Cheméo Relay (1.0)
log10ws	-9.29		Cheméo Relay (1.0)
logp	10.234		Crippen Method
mcvol	412.820	ml/mol	McGowan Method
pc	710.73	kPa	Joback Method
tb	665.09	K	Cheméo Relay (1.0)
tc	867.09	K	Cheméo Relay (1.0)
tf	370.75	K	Cheméo Relay (1.0)
vc	1.620	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.89	J/mol×K	986.09	Joback Method
cpg	1488.13	J/mol×K	1027.55	Joback Method
cpg	1511.59	J/mol×K	1069.01	Joback Method
cpg	1533.41	J/mol×K	1110.47	Joback Method
cpg	1553.74	J/mol×K	1151.93	Joback Method

cpg	1572.71	J/mol×K	1193.39	Joback Method
cpg	1590.45	J/mol×K	1234.84	Joback Method
dvisc	0.0003594	Pa×s	516.07	Joback Method
dvisc	0.0001025	Pa×s	594.41	Joback Method
dvisc	0.0000392	Pa×s	672.74	Joback Method
dvisc	0.0000183	Pa×s	751.08	Joback Method
dvisc	0.0000099	Pa×s	829.42	Joback Method
dvisc	0.0000059	Pa×s	907.75	Joback Method
dvisc	0.0000038	Pa×s	986.09	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C506489&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

Legend

af: Acentric Factor

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume