Octyl palmitate

Inchi: InChI=1S/C24H48O2/c1-3-5-7-9-11-12-13-14-15-16-17-18-20-22-24(25)26-23-21-19-10-
InchiKey: OQILCOQZDHPEAZ-UHFFFAOYSA-N
Formula: C24H48O2
SMILES: CCCCCCCCCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 368.65
CAS: 29806-73-3

Physical Properties

Property code	Value	Unit	Source
af	1.1159		Cheméo Relay (1.0)
hf	-854.30	kJ/mol	Cheméo Relay (1.0)
hfus	60.70	kJ/mol	Joback Method
hvap	113.84	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-8.04		Cheméo Relay (1.0)
logp	8.371		Crippen Method
mcvol	356.460	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook
tb	619.67	K	Cheméo Relay (1.0)
tc	804.07	K	Cheméo Relay (1.0)
tf	305.58	K	Cheméo Relay (1.0)
vc	1.406	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.81	J/mol×K	824.81	Joback Method
cpg	1178.47	J/mol×K	855.64	Joback Method
cpg	1198.97	J/mol×K	886.48	Joback Method
cpg	1218.34	J/mol×K	917.31	Joback Method
cpg	1236.63	J/mol×K	948.14	Joback Method
cpg	1253.86	J/mol×K	978.97	Joback Method

cpg	1270.08	J/mol×K	1009.81	Joback Method
dvisc	0.0010603	Pa×s	432.40	Joback Method
dvisc	0.0004342	Pa×s	497.80	Joback Method
dvisc	0.0002188	Pa×s	563.20	Joback Method
dvisc	0.0001271	Pa×s	628.61	Joback Method
dvisc	0.0000818	Pa×s	694.01	Joback Method
dvisc	0.0000568	Pa×s	759.41	Joback Method
dvisc	0.0000418	Pa×s	824.81	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.51615e+01
Coeff. B	-1.07086e+04
Coeff. C	-1.50804e+02
Temperature range (K), min.	581.32
Temperature range (K), max.	690.28

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C16958853&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

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume