Hexacosanol, acetate

Other names: n-Hexacosyl acetate
Acetic acid, hexacosyl ester
Cetyl alcohol acetate
Inchi: InChI=1S/C28H56O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-2
InchiKey: TXJQEFZXBSKQGU-UHFFFAOYSA-N
Formula: C28H56O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCOC(C)=O
Mol. weight [g/mol]: 424.75

Physical Properties

Property code	Value	Unit	Source
af	1.2460		Cheméo Relay (1.0)
gf	-49.04	kJ/mol	Joback Method
hf	-949.36	kJ/mol	Cheméo Relay (1.0)
hfus	71.06	kJ/mol	Joback Method
hvap	143.10	kJ/mol	Cheméo Relay (1.0)
ie	10.03	eV	Cheméo Relay (1.0)
log10ws	-9.34		Cheméo Relay (1.0)
logp	9.932		Crippen Method
mcvol	412.820	ml/mol	McGowan Method
pc	671.16	kPa	Joback Method
rinpol	2995.60		NIST Webbook
rinpol	2995.60		NIST Webbook
rinpol	3010.10		NIST Webbook
tb	645.40	K	Cheméo Relay (1.0)
tc	827.09	K	Cheméo Relay (1.0)
tf	332.53	K	Cheméo Relay (1.0)
vc	1.632	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1416.23	J/mol×K	916.33	Joback Method
cpg	1540.54	J/mol×K	1129.21	Joback Method

cpg	1523.34	J/mol×K	1093.73	Joback Method
cpg	1504.83	J/mol×K	1058.25	Joback Method
cpg	1484.93	J/mol×K	1022.77	Joback Method
cpg	1463.57	J/mol×K	987.29	Joback Method
cpg	1440.70	J/mol×K	951.81	Joback Method
dvisc	0.0000717	Pa×s	696.90	Joback Method
dvisc	0.0000230	Pa×s	916.33	Joback Method
dvisc	0.0000314	Pa×s	843.19	Joback Method
dvisc	0.0000457	Pa×s	770.05	Joback Method
dvisc	0.0006385	Pa×s	477.48	Joback Method
dvisc	0.0001253	Pa×s	623.76	Joback Method
dvisc	0.0002539	Pa×s	550.62	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C822322&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

rinpol: Non-polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume