Cetyl isooctanoate

Inchi: InChI=1S/C24H48O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-26-24(25)21-18-17-20
InchiKey: OIKBVOIOVNEVJR-UHFFFAOYSA-N
Formula: C24H48O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCC(C)C
Mol. weight [g/mol]: 368.64

Physical Properties

Property code	Value	Unit	Source
gf	-85.16	kJ/mol	Joback Method
hf	-788.77	kJ/mol	Joback Method
hfus	57.18	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	8.227		Crippen Method
mcvol	356.460	ml/mol	McGowan Method
pc	831.46	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	824.37	K	Joback Method
tc	1009.38	K	Joback Method
tf	417.40	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.23	J/mol×K	824.37	Joback Method
cpg	1254.21	J/mol×K	978.55	Joback Method
cpg	1237.01	J/mol×K	947.71	Joback Method
cpg	1218.75	J/mol×K	916.88	Joback Method
cpg	1199.39	J/mol×K	886.04	Joback Method
cpg	1178.90	J/mol×K	855.21	Joback Method
cpg	1270.38	J/mol×K	1009.38	Joback Method
dvisc	0.0000384	Pa×s	824.37	Joback Method

dvisc	0.0000530	Pa×s	756.54	Joback Method
dvisc	0.0000781	Pa×s	688.71	Joback Method
dvisc	0.0001252	Pa×s	620.88	Joback Method
dvisc	0.0002254	Pa×s	553.06	Joback Method
dvisc	0.0004783	Pa×s	485.23	Joback Method
dvisc	0.0012961	Pa×s	417.40	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=R44491&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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