Citronellyl palmitoleate

Inchi: InChI=1S/C26H48O2/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21-26(27)28-23-22-25(4)20
InchiKey: ZHXFNDSMLZVRDU-KHPPLWFESA-N
Formula: C26H48O2
SMILES: CCCCCCC=CCCCCCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 392.66

Physical Properties

Property code	Value	Unit	Source
gf	83.57	kJ/mol	Joback Method
hf	-605.40	kJ/mol	Joback Method
hfus	61.45	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.559		Crippen Method
mcvol	376.040	ml/mol	McGowan Method
pc	793.05	kPa	Joback Method
rinpol	2696.90		NIST Webbook
rinpol	2696.90		NIST Webbook
tb	878.33	K	Joback Method
tc	1075.33	K	Joback Method
tf	415.82	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1233.02	J/mol×K	878.33	Joback Method
cpg	1254.57	J/mol×K	911.16	Joback Method
cpg	1274.96	J/mol×K	944.00	Joback Method
cpg	1294.29	J/mol×K	976.83	Joback Method
cpg	1312.61	J/mol×K	1009.66	Joback Method
cpg	1329.99	J/mol×K	1042.50	Joback Method
cpg	1346.52	J/mol×K	1075.33	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U414430&Units=SI

Legend

cpg:	Ideal gas heat capacity
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