Adipic acid, «beta»-citronellyl dodecyl ester

Inchi: InChI=1S/C28H52O4/c1-5-6-7-8-9-10-11-12-13-16-23-31-27(29)20-14-15-21-28(30)32-2
InchiKey: IQLYIJFJWLLGEX-UHFFFAOYSA-N
Formula: C28H52O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-213.73	kJ/mol	Joback Method
hf	-1008.70	kJ/mol	Joback Method
hfus	69.22	kJ/mol	Joback Method
hvap	95.88	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	8.327		Crippen Method
mcvol	415.960	ml/mol	McGowan Method
pc	711.49	kPa	Joback Method
rinpol	3066.00		NIST Webbook
rinpol	3066.00		NIST Webbook
tb	996.22	K	Joback Method
tc	1230.18	K	Joback Method
tf	515.60	K	Joback Method
vc	1.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.41	J/mol×K	996.22	Joback Method
cpg	1468.21	J/mol×K	1035.21	Joback Method
cpg	1488.26	J/mol×K	1074.21	Joback Method
cpg	1506.66	J/mol×K	1113.20	Joback Method
cpg	1523.48	J/mol×K	1152.19	Joback Method
cpg	1538.81	J/mol×K	1191.19	Joback Method
cpg	1552.74	J/mol×K	1230.18	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=U353775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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