Adipic acid, «beta»-citronellyl undecyl ester

Inchi: InChI=1S/C27H50O4/c1-5-6-7-8-9-10-11-12-15-22-30-26(28)19-13-14-20-27(29)31-23-2
InchiKey: WHAUZJIEYLDUJL-UHFFFAOYSA-N
Formula: C27H50O4
SMILES: CCCCCCCCCCCOC(=O)CCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 438.68

Physical Properties

Property code	Value	Unit	Source
gf	-222.15	kJ/mol	Joback Method
hf	-988.06	kJ/mol	Joback Method
hfus	66.63	kJ/mol	Joback Method
hvap	93.66	kJ/mol	Joback Method
log10ws	-8.46		Crippen Method
logp	7.937		Crippen Method
mcvol	401.870	ml/mol	McGowan Method
pc	749.38	kPa	Joback Method
rinpol	2962.00		NIST Webbook
rinpol	2962.00		NIST Webbook
tb	973.34	K	Joback Method
tc	1197.78	K	Joback Method
tf	504.33	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.77	J/mol×K	973.34	Joback Method
cpg	1402.91	J/mol×K	1010.75	Joback Method
cpg	1422.45	J/mol×K	1048.15	Joback Method
cpg	1440.45	J/mol×K	1085.56	Joback Method
cpg	1456.99	J/mol×K	1122.97	Joback Method
cpg	1472.15	J/mol×K	1160.37	Joback Method
cpg	1485.98	J/mol×K	1197.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353774&Units=SI
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

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