Adipic acid, «beta»-citronellyl octyl ester

Inchi: InChI=1S/C24H44O4/c1-5-6-7-8-9-12-19-27-23(25)16-10-11-17-24(26)28-20-18-22(4)15
InchiKey: MXVHMEMSTPCEMA-UHFFFAOYSA-N
Formula: C24H44O4
SMILES: CCCCCCCCOC(=O)CCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 396.60

Physical Properties

Property code	Value	Unit	Source
gf	-247.41	kJ/mol	Joback Method
hf	-926.14	kJ/mol	Joback Method
hfus	58.86	kJ/mol	Joback Method
hvap	86.98	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.766		Crippen Method
mcvol	359.600	ml/mol	McGowan Method
pc	883.14	kPa	Joback Method
rinpol	2673.00		NIST Webbook
tb	904.70	K	Joback Method
tc	1107.69	K	Joback Method
tf	470.52	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.58	J/mol×K	904.70	Joback Method
cpg	1210.08	J/mol×K	938.53	Joback Method
cpg	1228.28	J/mol×K	972.36	Joback Method
cpg	1245.25	J/mol×K	1006.20	Joback Method
cpg	1261.03	J/mol×K	1040.03	Joback Method
cpg	1275.65	J/mol×K	1073.86	Joback Method
cpg	1289.17	J/mol×K	1107.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353772&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

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