Adipic acid, di(«beta»-citronellyl) ester

Inchi: InChI=1S/C26H46O4/c1-21(2)11-9-13-23(5)17-19-29-25(27)15-7-8-16-26(28)30-20-18-2
InchiKey: JYCAVOFTMMNBEY-UHFFFAOYSA-N
Formula: C26H46O4
SMILES: CC(C)=CCCC(C)CCOC(=O)CCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-161.34	kJ/mol	Joback Method
hf	-865.27	kJ/mol	Joback Method
hfus	59.41	kJ/mol	Joback Method
hvap	91.08	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	7.178		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	820.07	kPa	Joback Method
rinpol	2827.00		NIST Webbook
tb	954.06	K	Joback Method
tc	1168.64	K	Joback Method
tf	459.02	K	Joback Method
vc	1.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.78	J/mol×K	954.06	Joback Method
cpg	1309.68	J/mol×K	989.82	Joback Method
cpg	1328.27	J/mol×K	1025.59	Joback Method
cpg	1345.61	J/mol×K	1061.35	Joback Method
cpg	1361.78	J/mol×K	1097.11	Joback Method
cpg	1376.86	J/mol×K	1132.88	Joback Method
cpg	1390.92	J/mol×K	1168.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353780&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

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