Adipic acid, «beta»-citronellyl isohexyl ester

Inchi: InChI=1S/C22H40O4/c1-18(2)10-8-12-20(5)15-17-26-22(24)14-7-6-13-21(23)25-16-9-11
InchiKey: WKQAMVXEHVRFKC-UHFFFAOYSA-N
Formula: C22H40O4
SMILES: CC(C)=CCCC(C)CCOC(=O)CCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-266.69	kJ/mol	Joback Method
hf	-890.14	kJ/mol	Joback Method
hfus	50.16	kJ/mol	Joback Method
hvap	82.14	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.842		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	998.28	kPa	Joback Method
rinpol	2440.00		NIST Webbook
tb	858.50	K	Joback Method
tc	1052.82	K	Joback Method
tf	432.98	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.36	J/mol×K	858.50	Joback Method
cpg	1085.02	J/mol×K	890.89	Joback Method
cpg	1102.52	J/mol×K	923.27	Joback Method
cpg	1118.90	J/mol×K	955.66	Joback Method
cpg	1134.21	J/mol×K	988.05	Joback Method
cpg	1148.47	J/mol×K	1020.43	Joback Method
cpg	1161.71	J/mol×K	1052.82	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=U353769&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