Adipic acid, «beta»-citronellyl propyl ester

Inchi: InChI=1S/C19H34O4/c1-5-14-22-18(20)11-6-7-12-19(21)23-15-13-17(4)10-8-9-16(2)3/h9
InchiKey: JGZDRQVWOPDJRK-UHFFFAOYSA-N
Formula: C19H34O4
SMILES: CCCOC(=O)CCCCC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-289.51	kJ/mol	Joback Method
hf	-822.94	kJ/mol	Joback Method
hfus	45.91	kJ/mol	Joback Method
hvap	75.85	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.816		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1201.46	kPa	Joback Method
rinpol	2181.00		NIST Webbook
tb	790.30	K	Joback Method
tc	976.49	K	Joback Method
tf	414.17	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.21	J/mol×K	790.30	Joback Method
cpg	901.71	J/mol×K	821.33	Joback Method
cpg	918.23	J/mol×K	852.36	Joback Method
cpg	933.81	J/mol×K	883.40	Joback Method
cpg	948.46	J/mol×K	914.43	Joback Method
cpg	962.21	J/mol×K	945.46	Joback Method
cpg	975.09	J/mol×K	976.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353765&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

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