(E)-nuciferyl 2-methylpropanoate

Inchi: InChI=1S/C18H26O2/c1-14(2)18(19)20-13-15(3)9-8-10-16(4)17-11-6-5-7-12-17/h5-7,9,1
InchiKey: RDCVUVRTJSALNC-OQLLNIDSSA-N
Formula: C18H26O2
SMILES: CC(=CCCC(C)c1ccccc1)COC(=O)C(C)C
Mol. weight [g/mol]: 274.40

Physical Properties

Property code	Value	Unit	Source
gf	45.96	kJ/mol	Joback Method
hf	-326.25	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	66.36	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.716		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	1992.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	1992.00		NIST Webbook
tb	717.37	K	Joback Method
tc	924.40	K	Joback Method
tf	342.16	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.45	J/mol×K	717.37	Joback Method
cpg	706.57	J/mol×K	751.87	Joback Method
cpg	723.58	J/mol×K	786.38	Joback Method
cpg	739.52	J/mol×K	820.88	Joback Method
cpg	754.45	J/mol×K	855.39	Joback Method
cpg	768.42	J/mol×K	889.89	Joback Method
cpg	781.48	J/mol×K	924.40	Joback Method

Sources

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=R420356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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