(E)-nuciferyl formate

Inchi: InChI=1S/C16H22O2/c1-14-8-10-16(11-9-14)7-5-3-4-6-15(2)12-18-13-17/h6,8-11,13H,3-
InchiKey: LIGLXUWLWGOJKZ-GIDUJCDVSA-N
Formula: C16H22O2
SMILES: CC(=CCCCCc1ccc(C)cc1)COC=O
Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	53.77	kJ/mol	Joback Method
hf	-258.88	kJ/mol	Joback Method
hfus	33.22	kJ/mol	Joback Method
hvap	63.32	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.827		Crippen Method
mcvol	215.680	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1777.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1775.00		NIST Webbook
tb	672.26	K	Joback Method
tc	874.43	K	Joback Method
tf	354.21	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.18	J/mol×K	672.26	Joback Method
cpg	593.64	J/mol×K	705.95	Joback Method
cpg	609.16	J/mol×K	739.65	Joback Method
cpg	623.77	J/mol×K	773.34	Joback Method
cpg	637.52	J/mol×K	807.04	Joback Method
cpg	650.46	J/mol×K	840.73	Joback Method
cpg	662.60	J/mol×K	874.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R232852&Units=SI

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