(E)-nuciferyl butanoate

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

Physical Properties

Property code	Value	Unit	Source
gf	48.40	kJ/mol	Joback Method
hf	-320.97	kJ/mol	Joback Method
hfus	34.57	kJ/mol	Joback Method
hvap	66.74	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.860		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2004.00		NIST Webbook
tb	717.81	K	Joback Method
tc	921.52	K	Joback Method
tf	357.16	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.95	J/mol×K	717.81	Joback Method
cpg	705.77	J/mol×K	751.76	Joback Method
cpg	722.51	J/mol×K	785.71	Joback Method
cpg	738.23	J/mol×K	819.67	Joback Method
cpg	752.98	J/mol×K	853.62	Joback Method
cpg	766.81	J/mol×K	887.57	Joback Method
cpg	779.76	J/mol×K	921.52	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=R420361&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