Nuciferyl acetate

Other names: n-Nuciferyl acetate
Inchi: InChI=1S/C17H24O2/c1-14-9-11-17(12-10-14)8-6-4-5-7-15(2)13-19-16(3)18/h7,9-12H,4-
InchiKey: BWLPFSJVSUPCNH-UHFFFAOYSA-N
Formula: C17H24O2
SMILES: CC(=O)OCC(C)=CCCCCc1ccc(C)cc1
Mol. weight [g/mol]: 260.37

Physical Properties

Property code	Value	Unit	Source
gf	32.79	kJ/mol	Joback Method
hf	-306.52	kJ/mol	Joback Method
hfus	35.12	kJ/mol	Joback Method
hvap	65.57	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.217		Crippen Method
mcvol	229.770	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1830.00		NIST Webbook
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tb	700.35	K	Joback Method
tc	903.88	K	Joback Method
tf	373.41	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.58	J/mol×K	700.35	Joback Method
cpg	648.67	J/mol×K	734.27	Joback Method
cpg	664.77	J/mol×K	768.19	Joback Method
cpg	679.92	J/mol×K	802.12	Joback Method
cpg	694.16	J/mol×K	836.04	Joback Method
cpg	707.53	J/mol×K	869.96	Joback Method
cpg	720.07	J/mol×K	903.88	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=R203879&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