(E)-Nuciferyl 2-methylbutyrate

Inchi: InChI=1S/C20H30O2/c1-5-18(4)20(21)22-15-17(3)9-7-6-8-10-19-13-11-16(2)12-14-19/h9
InchiKey: GFHTTYIWKJYNHU-RQZCQDPDSA-N
Formula: C20H30O2
SMILES: CCC(C)C(=O)OCC(C)=CCCCCc1ccc(C)cc1
Mol. weight [g/mol]: 302.45

Physical Properties

Property code	Value	Unit	Source
gf	55.61	kJ/mol	Joback Method
hf	-373.72	kJ/mol	Joback Method
hfus	39.36	kJ/mol	Joback Method
hvap	71.86	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.243		Crippen Method
mcvol	272.040	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	2075.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2081.00		NIST Webbook
rinpol	2101.00		NIST Webbook
tb	768.55	K	Joback Method
tc	969.63	K	Joback Method
tf	392.22	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.80	J/mol×K	768.55	Joback Method
cpg	819.94	J/mol×K	802.06	Joback Method
cpg	837.00	J/mol×K	835.58	Joback Method
cpg	853.04	J/mol×K	869.09	Joback Method
cpg	868.10	J/mol×K	902.60	Joback Method
cpg	882.24	J/mol×K	936.11	Joback Method

cpg	895.49	J/mol×K	969.63	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=R233068&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