(Z)-Nuciferyl isobutyrate

Inchi: InChI=1S/C19H28O2/c1-5-7-19(20)21-14-16(3)8-6-9-17(4)18-12-10-15(2)11-13-18/h8,10
InchiKey: PPVOLQCPZBGHKH-PXNMLYILSA-N
Formula: C19H28O2
SMILES: CCCC(=O)OCC(C)=CCCC(C)c1ccc(C)cc1
Mol. weight [g/mol]: 288.42

Physical Properties

Property code	Value	Unit	Source
hfus	36.77	kJ/mol	Joback Method
ie	8.02	eV	Cheméo Relay (1.0)
logp	5.168		Crippen Method
mcvol	257.950	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.16	J/mol×K	745.67	Joback Method
cpg	762.09	J/mol×K	779.43	Joback Method
cpg	778.95	J/mol×K	813.19	Joback Method
cpg	794.80	J/mol×K	846.94	Joback Method
cpg	809.68	J/mol×K	880.70	Joback Method
cpg	823.64	J/mol×K	914.46	Joback Method
cpg	836.72	J/mol×K	948.22	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R615400&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume