(Z)-Nuciferyl isobutyrate

Inchi: InChI=1S/C19H28O2/c1-15(2)19(20)21-14-17(4)8-6-5-7-9-18-12-10-16(3)11-13-18/h8,10
InchiKey: PNFRTFPRRKETBY-IUXPMGMMSA-N
Formula: C19H28O2
SMILES: CC(=CCCCCc1ccc(C)cc1)COC(=O)C(C)C
Mol. weight [g/mol]: 288.42

Physical Properties

Property code	Value	Unit	Source
hfus	36.77	kJ/mol	Joback Method
logp	4.853		Crippen Method
mcvol	257.950	ml/mol	McGowan Method
rinpol	1945.00		NIST Webbook
rinpol	1935.00		NIST Webbook
rinpol	1934.00		NIST Webbook
rinpol	1945.00		NIST Webbook
tf	275.20	K	Cheméo Relay (1.0)

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

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233360&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point