Neryl benzoate

Inchi: InChI=1S/C18H24O2/c1-15(2)9-7-10-16(3)11-8-14-20-18(19)17-12-5-4-6-13-17/h4-6,9,1
InchiKey: LWTRZPZIWZJTIG-WJDWOHSUSA-N
Formula: C18H24O2
SMILES: CC(C)=CCCC(C)=CCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	122.51	kJ/mol	Joback Method
hf	-208.26	kJ/mol	Joback Method
hfus	36.99	kJ/mol	Joback Method
hvap	67.17	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.926		Crippen Method
mcvol	239.560	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
ripol	2586.00		NIST Webbook
ripol	2586.00		NIST Webbook
tb	722.29	K	Joback Method
tc	932.40	K	Joback Method
tf	353.12	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.77	J/mol×K	722.29	Joback Method
cpg	681.03	J/mol×K	757.31	Joback Method
cpg	697.23	J/mol×K	792.33	Joback Method
cpg	712.44	J/mol×K	827.34	Joback Method
cpg	726.73	J/mol×K	862.36	Joback Method
cpg	740.17	J/mol×K	897.38	Joback Method
cpg	752.81	J/mol×K	932.40	Joback Method

Sources

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=R328191&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume