NERYL PHENYLACETATE

Other names: Phenyl (4Z)-5,9-dimethyl-4,8-decadienoate
Inchi: InChI=1S/C18H24O2/c1-15(2)9-7-10-16(3)11-8-14-18(19)20-17-12-5-4-6-13-17/h4-6,9,1
InchiKey: PCXFODQCJDGIDX-WJDWOHSUSA-N
Formula: C18H24O2
SMILES: CC(C)=CCC/C(C)=C\CCC(=O)Oc1ccccc1
Mol. weight [g/mol]: 272.39

Physical Properties

Property code	Value	Unit	Source
hf	-334.42	kJ/mol	Cheméo Relay (1.0)
hfus	36.99	kJ/mol	Joback Method
hvap	85.72	kJ/mol	Cheméo Relay (1.0)
ie	8.07	eV	Cheméo Relay (1.0)
log10ws	-5.14		Cheméo Relay (1.0)
logp	5.065		Crippen Method
mcvol	239.560	ml/mol	McGowan Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook
tb	594.34	K	Cheméo Relay (1.0)
tf	272.02	K	Cheméo Relay (1.0)

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

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=U109594&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point