

Neryl methacrylate

Inchi:	InChI=1S/C14H22O2/c1-11(2)7-6-8-13(5)9-10-16-14(15)12(3)4/h7,9H,3,6,8,10H2,1-2,4-5
InchiKey:	DWJIEXRXQKFNAB-LCYFTJDESA-N
Formula:	C14H22O2
SMILES:	C=C(C)C(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	222.32

Physical Properties

Property code	Value	Unit	Source
gf	55.71	kJ/mol	Joback Method
hf	-246.59	kJ/mol	Joback Method
hfus	30.00	kJ/mol	Joback Method
hvap	55.40	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.798		Crippen Method
mcvol	202.660	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
ripol	1857.00		NIST Webbook
tb	600.65	K	Joback Method
tc	792.36	K	Joback Method
tf	265.90	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.56	J/molxK	600.65	Joback Method
cpg	521.78	J/molxK	632.60	Joback Method
cpg	537.16	J/molxK	664.55	Joback Method
cpg	551.76	J/molxK	696.51	Joback Method
cpg	565.60	J/molxK	728.46	Joback Method
cpg	578.73	J/molxK	760.41	Joback Method
cpg	591.18	J/molxK	792.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R518235&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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