Neryl tiglate

Inchi: InChI=1S/C15H24O2/c1-6-14(5)15(16)17-11-10-13(4)9-7-8-12(2)3/h6,8,10H,7,9,11H2,1-
InchiKey: OGHBUHJLMHQMHS-FVJRQPFYSA-N
Formula: C15H24O2
SMILES: CC=C(C)C(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	56.51	kJ/mol	Joback Method
hf	-275.44	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.189		Crippen Method
mcvol	216.750	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	1652.00		NIST Webbook
ripol	2054.00		NIST Webbook
ripol	2054.00		NIST Webbook
tb	631.01	K	Joback Method
tc	824.40	K	Joback Method
tf	273.85	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.71	J/mol×K	631.01	Joback Method
cpg	575.50	J/mol×K	663.24	Joback Method
cpg	591.43	J/mol×K	695.47	Joback Method
cpg	606.52	J/mol×K	727.71	Joback Method
cpg	620.85	J/mol×K	759.94	Joback Method
cpg	634.44	J/mol×K	792.17	Joback Method
cpg	647.37	J/mol×K	824.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R417251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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