Neryl heptanoate

Other names: Neryl-n-heptanoate
Inchi: InChI=1S/C17H30O2/c1-5-6-7-8-12-17(18)19-14-13-16(4)11-9-10-15(2)3/h10,13H,5-9,11
InchiKey: NSMHPPLPBQPIQJ-SSZFMOIBSA-N
Formula: C17H30O2
SMILES: CCCCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 266.42

Physical Properties

Property code	Value	Unit	Source
gf	1.68	kJ/mol	Joback Method
hf	-424.15	kJ/mol	Joback Method
hfus	40.36	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.193		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1808.00		NIST Webbook
ripol	2120.00		NIST Webbook
ripol	2120.00		NIST Webbook
tb	672.73	K	Joback Method
tc	854.15	K	Joback Method
tf	315.43	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.75	J/mol×K	672.73	Joback Method
cpg	706.58	J/mol×K	702.97	Joback Method
cpg	723.56	J/mol×K	733.20	Joback Method

cpg	739.73	J/mol×K	763.44	Joback Method
cpg	755.11	J/mol×K	793.68	Joback Method
cpg	769.75	J/mol×K	823.92	Joback Method
cpg	783.68	J/mol×K	854.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R289462&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