

Neryl hexanoate

Inchi:	InChI=1S/C16H28O2/c1-5-6-7-11-16(17)18-13-12-15(4)10-8-9-14(2)3/h9,12H,5-8,10-11,
InchiKey:	ARVSCQUZFFSNKF-QINSGFPZSA-N
Formula:	C16H28O2
SMILES:	CCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	252.39
CAS:	68310-59-8

Physical Properties

Property code	Value	Unit	Source
gf	-6.74	kJ/mol	Joback Method
hf	-403.51	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	60.44	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.803		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1709.00		NIST Webbook
rinpol	1732.10		NIST Webbook
rinpol	1732.10		NIST Webbook
ripol	2021.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2021.00		NIST Webbook
ripol	2031.00		NIST Webbook
ripol	2031.00		NIST Webbook
ripol	2033.00		NIST Webbook
ripol	2033.00		NIST Webbook
tb	649.85	K	Joback Method
tc	832.31	K	Joback Method
tf	304.16	K	Joback Method
vc	0.917	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.54	J/mol×K	649.85	Joback Method
cpg	650.98	J/mol×K	680.26	Joback Method
cpg	667.59	J/mol×K	710.67	Joback Method
cpg	683.39	J/mol×K	741.08	Joback Method
cpg	698.43	J/mol×K	771.49	Joback Method
cpg	712.73	J/mol×K	801.90	Joback Method
cpg	726.35	J/mol×K	832.31	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=C68310598&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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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