

Neryl valerate

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H26O2/c1-5-6-10-15(16)17-12-11-14(4)9-7-8-13(2)3/h8,11H,5-7,9-10,12H2

CVSWGLSBJFKWMW-KAMYIIQDSA-N

C15H26O2

CCCCC(=O)OCC=C(C)CCC=C(C)C

238.37

Physical Properties

Property code	Value	Unit	Source
gf	-15.16	kJ/mol	Joback Method
hf	-382.87	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	58.22	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.412		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
ripol	1618.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1930.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1933.00		NIST Webbook
ripol	1974.00		NIST Webbook
ripol	1933.00		NIST Webbook
tb	626.97	K	Joback Method
tc	810.82	K	Joback Method
tf	292.89	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.64	J/mol×K	626.97	Joback Method

cpg	596.65	J/mol×K	657.61	Joback Method
cpg	612.84	J/mol×K	688.25	Joback Method
cpg	628.25	J/mol×K	718.90	Joback Method
cpg	642.90	J/mol×K	749.54	Joback Method
cpg	656.84	J/mol×K	780.18	Joback Method
cpg	670.10	J/mol×K	810.82	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241584&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
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

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