

Neryl isovalerate

Other names:	Neryl 3-methylbutanoate Neryl 3-methylbutyrate
Inchi:	InChI=1S/C15H26O2/c1-12(2)7-6-8-14(5)9-10-17-15(16)11-13(3)4/h7,9,13H,6,8,10-11H2
InchiKey:	SOUKTGNMIRUIQN-ZROIWOOFSA-N
Formula:	C15H26O2
SMILES:	CC(C)=CCCC(C)=CCOC(=O)CC(C)C
Mol. weight [g/mol]:	238.37
CAS:	3915-83-1

Physical Properties

Property code	Value	Unit	Source
gf	-17.60	kJ/mol	Joback Method
hf	-388.15	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.268		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1576.00		NIST Webbook
rinpol	1565.00		NIST Webbook
rinpol	1566.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1587.90		NIST Webbook
rinpol	1576.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1587.90		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1560.00		NIST Webbook

ripol	1875.00		NIST Webbook
ripol	1877.00		NIST Webbook
ripol	1867.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1864.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1871.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1872.00		NIST Webbook
tb	626.53	K	Joback Method
tc	813.52	K	Joback Method
tf	277.89	K	Joback Method
vc	0.856	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.04	J/mol×K	626.53	Joback Method
cpg	597.38	J/mol×K	657.69	Joback Method
cpg	613.87	J/mol×K	688.86	Joback Method
cpg	629.53	J/mol×K	720.02	Joback Method
cpg	644.42	J/mol×K	751.19	Joback Method
cpg	658.56	J/mol×K	782.35	Joback Method
cpg	671.98	J/mol×K	813.52	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C3915831&Units=SI>

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

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

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