

Neryl isobutanoate

Other names:	Neryl isobutyrate neryl 2-methylpropanoate
Inchi:	InChI=1S/C14H24O2/c1-11(2)7-6-8-13(5)9-10-16-14(15)12(3)4/h7,9,12H,6,8,10H2,1-5H3
InchiKey:	OGJYXQFXLSCKTP-LCYFTJDESA-N
Formula:	C14H24O2
SMILES:	CC(C)=CCCC(C)=CCOC(=O)C(C)C
Mol. weight [g/mol]:	224.34
CAS:	2345-24-6

Physical Properties

Property code	Value	Unit	Source
gf	-26.02	kJ/mol	Joback Method
hf	-367.51	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	55.60	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.878		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1485.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1486.60		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1486.60		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1772.00		NIST Webbook

ripol	1761.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1766.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1766.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1769.00		NIST Webbook
ripol	1780.00		NIST Webbook
tb	603.65	K	Joback Method
tc	792.58	K	Joback Method
tf	266.62	K	Joback Method
vc	0.799	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.51	J/mol×K	603.65	Joback Method
cpg	544.38	J/mol×K	635.14	Joback Method
cpg	560.42	J/mol×K	666.63	Joback Method
cpg	575.66	J/mol×K	698.11	Joback Method
cpg	590.12	J/mol×K	729.60	Joback Method
cpg	603.86	J/mol×K	761.09	Joback Method
cpg	616.90	J/mol×K	792.58	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=C2345246&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
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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