Neryl formate

Other names: 2,6-Octadien-1-ol, 3,7-dimethyl-, formate, (Z)-
3,7-Dimethyl-cis-2,6-octadienyl formate
Inchi: InChI=1S/C11H18O2/c1-10(2)5-4-6-11(3)7-8-13-9-12/h5,7,9H,4,6,8H2,1-3H3/b11-7-
InchiKey: FQMZVFJYMPNUCT-XFFZJAGNSA-N
Formula: C11H18O2
SMILES: CC(C)=CCCC(C)=CCOC=O
Mol. weight [g/mol]: 182.26
CAS: 2142-94-1

Physical Properties

Property code	Value	Unit	Source
gf	-19.44	kJ/mol	Joback Method
hf	-273.31	kJ/mol	Joback Method
hfus	25.51	kJ/mol	Joback Method
hvap	49.29	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.852		Crippen Method
mcvol	164.690	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1261.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1284.10		NIST Webbook
rinpol	1284.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1268.00		NIST Webbook

rinpol	1267.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1267.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1641.00		NIST Webbook
ripol	1708.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1663.00		NIST Webbook
ripol	1663.00		NIST Webbook
tb	530.24	K	Joback Method
tc	717.87	K	Joback Method
tf	239.88	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.50	J/mol×K	530.24	Joback Method
cpg	393.81	J/mol×K	561.51	Joback Method
cpg	407.43	J/mol×K	592.78	Joback Method
cpg	420.37	J/mol×K	624.05	Joback Method
cpg	432.67	J/mol×K	655.33	Joback Method
cpg	444.36	J/mol×K	686.60	Joback Method
cpg	455.48	J/mol×K	717.87	Joback Method
hvapt	58.10	kJ/mol	414.00	NIST Webbook

Sources

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=C2142941&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt:	Enthalpy of vaporization at a given temperature
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