Neryl butyrate

Other names: Neryl butanoate
Inchi: InChI=1S/C14H24O2/c1-5-7-14(15)16-11-10-13(4)9-6-8-12(2)3/h8,10H,5-7,9,11H2,1-4H
InchiKey: ZSBOMYJPSRFZAL-RAXLEYEMSA-N
Formula: C14H24O2
SMILES: CCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 224.34
CAS: 999-40-6

Physical Properties

Property code	Value	Unit	Source
gf	-23.58	kJ/mol	Joback Method
hf	-362.23	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	55.99	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.022		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1514.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1498.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1828.00		NIST Webbook
ripol	1857.00		NIST Webbook
tb	604.09	K	Joback Method
tc	789.66	K	Joback Method
tf	281.62	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.13	J/mol×K	604.09	Joback Method
cpg	543.66	J/mol×K	635.02	Joback Method
cpg	559.39	J/mol×K	665.95	Joback Method
cpg	574.35	J/mol×K	696.87	Joback Method
cpg	588.58	J/mol×K	727.80	Joback Method
cpg	602.10	J/mol×K	758.73	Joback Method
cpg	614.97	J/mol×K	789.66	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C999406&Units=SI
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

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