Ethyl nerate

Inchi: InChI=1S/C12H20O2/c1-5-14-12(13)9-11(4)8-6-7-10(2)3/h7,9H,5-6,8H2,1-4H3/b11-9-
InchiKey: ZPKNTCZTABQJPS-LUAWRHEFSA-N
Formula: C12H20O2
SMILES: CCOC(=O)C=C(C)CCC=C(C)C
Mol. weight [g/mol]: 196.29
CAS: 32659-20-4

Physical Properties

Property code	Value	Unit	Source
gf	-40.42	kJ/mol	Joback Method
hf	-320.95	kJ/mol	Joback Method
hfus	27.41	kJ/mol	Joback Method
hvap	51.54	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.242		Crippen Method
mcvol	178.780	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
ripol	1698.00		NIST Webbook
tb	558.33	K	Joback Method
tc	748.06	K	Joback Method
tf	259.08	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.65	J/mol×K	558.33	Joback Method
cpg	442.01	J/mol×K	589.95	Joback Method
cpg	456.62	J/mol×K	621.57	Joback Method
cpg	470.50	J/mol×K	653.20	Joback Method
cpg	483.69	J/mol×K	684.82	Joback Method
cpg	496.22	J/mol×K	716.44	Joback Method
cpg	508.12	J/mol×K	748.06	Joback Method

Sources

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=C32659204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume