(E)-Lyratyl propanoate

Inchi: InChI=1S/C13H20O2/c1-6-12(10(3)4)8-11(5)9-15-13(14)7-2/h6,8,12H,1,3,7,9H2,2,4-5H3
InchiKey: UYACSVLHQPEITQ-DHZHZOJOSA-N
Formula: C13H20O2
SMILES: C=CC(C=C(C)COC(=O)CC)C(=C)C
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	61.02	kJ/mol	Joback Method
hf	-213.23	kJ/mol	Joback Method
hfus	23.71	kJ/mol	Joback Method
hvap	52.08	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.264		Crippen Method
mcvol	188.570	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1583.00		NIST Webbook
rinpol	1583.00		NIST Webbook
tb	569.97	K	Joback Method
tc	760.45	K	Joback Method
tf	256.91	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.71	J/mol×K	569.97	Joback Method
cpg	470.38	J/mol×K	601.72	Joback Method
cpg	485.25	J/mol×K	633.46	Joback Method
cpg	499.37	J/mol×K	665.21	Joback Method
cpg	512.75	J/mol×K	696.96	Joback Method
cpg	525.44	J/mol×K	728.70	Joback Method
cpg	537.46	J/mol×K	760.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R342375&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume