(E)-2-Methyl-5-((1S,2R,4R)-2-methyl-3-methyleneb
acid

Inchi: InChI=1S/C15H22O2/c1-10(14(16)17)5-4-8-15(3)11(2)12-6-7-13(15)9-12/h5,12-13H,2,4,

InchiKey: PMCPDNGTLRPFQQ-BJMVGYQFSA-N

Formula: C15H22O2

SMILES: C=C1C2CCC(C2)C1(C)CCC=C(C)C(=O)O

Mol. weight [g/mol]: 234.33

CAS: 872880-61-0

Physical Properties

Property code	Value	Unit	Source
gf	30.63	kJ/mol	Joback Method
hf	-291.73	kJ/mol	Joback Method
hfus	26.97	kJ/mol	Joback Method
hvap	71.14	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.790		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	1886.90		NIST Webbook
rinpol	1886.90		NIST Webbook
tb	705.17	K	Joback Method
tc	905.75	K	Joback Method
tf	416.22	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.75	J/mol×K	705.17	Joback Method
cpg	602.31	J/mol×K	738.60	Joback Method
cpg	617.24	J/mol×K	772.03	Joback Method
cpg	631.68	J/mol×K	805.46	Joback Method
cpg	645.78	J/mol×K	838.89	Joback Method
cpg	659.68	J/mol×K	872.32	Joback Method
cpg	673.51	J/mol×K	905.75	Joback Method

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=C872880610&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
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