(1R,3R)-3-isopropenyl-2,2-dimethylcyclobutylmeth 3-methyl-3-butenoate

Inchi: InChI=1S/C15H24O2/c1-10(2)7-14(16)17-9-12-8-13(11(3)4)15(12,5)6/h12-13H,1,3,7-9H2

InchiKey: DYIOGDMFNJSASB-STQMWFEESA-N

Formula: C15H24O2

SMILES: C=C(C)CC(=O)OCC1CC(C(=C)C)C1(C)C

Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	27.82	kJ/mol	Joback Method
hf	-325.25	kJ/mol	Joback Method
hfus	24.09	kJ/mol	Joback Method
hvap	55.28	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.734		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	1526.00		NIST Webbook
ripol	1905.00		NIST Webbook
tb	613.92	K	Joback Method
tc	813.30	K	Joback Method
tf	329.37	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.85	J/mol×K	613.92	Joback Method
cpg	583.72	J/mol×K	647.15	Joback Method
cpg	601.64	J/mol×K	680.38	Joback Method
cpg	618.71	J/mol×K	713.61	Joback Method
cpg	635.03	J/mol×K	746.84	Joback Method
cpg	650.71	J/mol×K	780.07	Joback Method
cpg	665.83	J/mol×K	813.30	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=R504419&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
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

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