Fumaric acid, isobutyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C13H20O4/c1-10(2)7-8-16-12(14)5-6-13(15)17-9-11(3)4/h5-6,11H,1,7-9H2,2-4

InchiKey: PJWIMMPQOALWST-AATRIKPKSA-N

Formula: C13H20O4

SMILES: C=C(C)CCOC(=O)C=CC(=O)OCC(C)C

Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-252.19	kJ/mol	Joback Method
hf	-573.67	kJ/mol	Joback Method
hfus	29.09	kJ/mol	Joback Method
hvap	61.82	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.251		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1607.00		NIST Webbook
rinpol	1607.00		NIST Webbook
tb	649.70	K	Joback Method
tc	840.22	K	Joback Method
tf	344.79	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.52	J/mol×K	649.70	Joback Method
cpg	539.05	J/mol×K	681.45	Joback Method
cpg	552.83	J/mol×K	713.21	Joback Method
cpg	565.88	J/mol×K	744.96	Joback Method
cpg	578.22	J/mol×K	776.71	Joback Method
cpg	589.86	J/mol×K	808.47	Joback Method
cpg	600.83	J/mol×K	840.22	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=U348901&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