Fumaric acid, isobutyl pent-4-en-2-yl ester

Inchi: InChI=1S/C13H20O4/c1-5-6-11(4)17-13(15)8-7-12(14)16-9-10(2)3/h5,7-8,10-11H,1,6,9H
InchiKey: WXNYTZSPSXNNFE-BQYQJAHWSA-N
Formula: C13H20O4
SMILES: C=CCC(C)OC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-246.08	kJ/mol	Joback Method
hf	-569.16	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.250		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1552.00		NIST Webbook
tb	649.38	K	Joback Method
tc	840.40	K	Joback Method
tf	343.75	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.27	J/mol×K	649.38	Joback Method
cpg	539.89	J/mol×K	681.22	Joback Method
cpg	553.76	J/mol×K	713.05	Joback Method
cpg	566.88	J/mol×K	744.89	Joback Method
cpg	579.27	J/mol×K	776.72	Joback Method
cpg	590.95	J/mol×K	808.56	Joback Method
cpg	601.94	J/mol×K	840.40	Joback Method
dvisc	0.0023112	Pa×s	343.75	Joback Method
dvisc	0.0009902	Pa×s	394.69	Joback Method

dvisc	0.0005149	Pa×s	445.63	Joback Method
dvisc	0.0003062	Pa×s	496.56	Joback Method
dvisc	0.0002006	Pa×s	547.50	Joback Method
dvisc	0.0001412	Pa×s	598.44	Joback Method
dvisc	0.0001050	Pa×s	649.38	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=U348922&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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