Fumaric acid, 3,3-dimethylbut-2-yl isobutyl ester

Inchi: InChI=1S/C14H24O4/c1-10(2)9-17-12(15)7-8-13(16)18-11(3)14(4,5)6/h7-8,10-11H,9H2,1

InchiKey: GDOAQDJHOVUXRA-BQYQJAHWSA-N

Formula: C14H24O4

SMILES: CC(C)COC(=O)C=CC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-322.66	kJ/mol	Joback Method
hf	-723.98	kJ/mol	Joback Method
hfus	23.33	kJ/mol	Joback Method
hvap	62.96	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.720		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	1585.00		NIST Webbook
tb	672.35	K	Joback Method
tc	867.38	K	Joback Method
tf	359.20	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.73	J/mol×K	672.35	Joback Method
cpg	619.89	J/mol×K	704.86	Joback Method
cpg	635.14	J/mol×K	737.36	Joback Method
cpg	649.51	J/mol×K	769.87	Joback Method
cpg	663.02	J/mol×K	802.37	Joback Method
cpg	675.71	J/mol×K	834.88	Joback Method
cpg	687.62	J/mol×K	867.38	Joback Method
dvisc	0.0023705	Pa×s	359.20	Joback Method
dvisc	0.0009272	Pa×s	411.39	Joback Method

dvisc	0.0004480	Pa×s	463.58	Joback Method
dvisc	0.0002508	Pa×s	515.78	Joback Method
dvisc	0.0001562	Pa×s	567.97	Joback Method
dvisc	0.0001054	Pa×s	620.16	Joback Method
dvisc	0.0000756	Pa×s	672.35	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=U348701&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

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