

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,
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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0004480	Paxs	463.58	Joback Method
dvisc	0.0002508	Paxs	515.78	Joback Method
dvisc	0.0001562	Paxs	567.97	Joback Method
dvisc	0.0001054	Paxs	620.16	Joback Method
dvisc	0.0000756	Paxs	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
mccvol:	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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