

Fumaric acid, butyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C14H24O4/c1-5-7-10-17-13(15)8-9-14(16)18-12(6-2)11(3)4/h8-9,11-12H,5-7,1
InchiKey:	NWQVIURKKKITDZ-CMDGGOBGSA-N
Formula:	C14H24O4
SMILES:	CCCCOC(=O)C=CC(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-325.50	kJ/mol	Joback Method
hf	-715.23	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	64.25	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.864		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinsol	1671.00		NIST Webbook
tb	675.58	K	Joback Method
tc	862.18	K	Joback Method
tf	356.78	K	Joback Method
vc	0.836	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.07	J/molxK	675.58	Joback Method
cpg	616.74	J/molxK	706.68	Joback Method
cpg	631.60	J/molxK	737.78	Joback Method
cpg	645.68	J/molxK	768.88	Joback Method
cpg	658.99	J/molxK	799.98	Joback Method
cpg	671.55	J/molxK	831.08	Joback Method
cpg	683.37	J/molxK	862.18	Joback Method
dvisc	0.0021664	Paxs	356.78	Joback Method
dvisc	0.0009003	Paxs	409.91	Joback Method

dvisc	0.0004576	Paxs	463.05	Joback Method
dvisc	0.0002674	Paxs	516.18	Joback Method
dvisc	0.0001727	Paxs	569.31	Joback Method
dvisc	0.0001202	Paxs	622.45	Joback Method
dvisc	0.0000886	Paxs	675.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U348761&Units=SI

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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