

Fumaric acid, butyl 2-butyl ester

Inchi:	InChI=1S/C12H20O4/c1-4-6-9-15-11(13)7-8-12(14)16-10(3)5-2/h7-8,10H,4-6,9H2,1-3H3
InchiKey:	DWHTZZBOKCNKRP-BQYQJAHWSA-N
Formula:	C12H20O4
SMILES:	CCCCOC(=O)C=CC(=O)OC(C)CC
Mol. weight [g/mol]:	228.28

Physical Properties

Property code	Value	Unit	Source
gf	-339.90	kJ/mol	Joback Method
hf	-668.67	kJ/mol	Joback Method
hfus	29.09	kJ/mol	Joback Method
hvap	60.19	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.228		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1526.00		NIST Webbook
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tb	630.26	K	Joback Method
tc	816.90	K	Joback Method
tf	349.24	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.48	J/molxK	630.26	Joback Method
cpg	509.82	J/molxK	661.37	Joback Method
cpg	523.48	J/molxK	692.47	Joback Method
cpg	536.46	J/molxK	723.58	Joback Method
cpg	548.77	J/molxK	754.69	Joback Method
cpg	560.42	J/molxK	785.80	Joback Method
cpg	571.41	J/molxK	816.90	Joback Method
dvisc	0.0019896	Paxs	349.24	Joback Method

dvisc	0.0009475	Paxs	396.08	Joback Method
dvisc	0.0005279	Paxs	442.91	Joback Method
dvisc	0.0003289	Paxs	489.75	Joback Method
dvisc	0.0002226	Paxs	536.59	Joback Method
dvisc	0.0001604	Paxs	583.42	Joback Method
dvisc	0.0001213	Paxs	630.26	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=U348640&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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