

Fumaric acid, 2-butyl octyl ester

Inchi:	InChI=1S/C16H28O4/c1-4-6-7-8-9-10-13-19-15(17)11-12-16(18)20-14(3)5-2/h11-12,14H
InchiKey:	XKPMRKINMLLCMX-VAWYXSNFSA-N
Formula:	C16H28O4
SMILES:	CCCCCCCCOC(=O)C=CC(=O)OC(C)CC
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-306.22	kJ/mol	Joback Method
hf	-751.23	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.788		Crippen Method
mvol	246.880	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	1928.00		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	721.78	K	Joback Method
tc	904.51	K	Joback Method
tf	394.32	K	Joback Method
vc	0.954	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.90	J/molxK	721.78	Joback Method
cpg	727.17	J/molxK	752.23	Joback Method
cpg	742.59	J/molxK	782.69	Joback Method
cpg	757.19	J/molxK	813.14	Joback Method
cpg	770.99	J/molxK	843.60	Joback Method
cpg	783.99	J/molxK	874.05	Joback Method
cpg	796.23	J/molxK	904.51	Joback Method
dvisc	0.0014186	Paxs	394.32	Joback Method

dvisc	0.0006427	Paxs	448.90	Joback Method
dvisc	0.0003457	Paxs	503.47	Joback Method
dvisc	0.0002100	Paxs	558.05	Joback Method
dvisc	0.0001394	Paxs	612.63	Joback Method
dvisc	0.0000989	Paxs	667.20	Joback Method
dvisc	0.0000739	Paxs	721.78	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=U348645&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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