

2-Butenedioic acid (E)-, bis(2-ethylhexyl) ester

Other names:	Fumaric acid, bis(2-ethylhexyl) ester Bis(2-ethylhexyl) fumarate DOF RC Comonomer DOF 2-Ethylhexyl fumarate Bis-(2-ethylhexyl)ester kyseliny fumarove 2-Butenedioic acid, bis(2-ethylhexyl) ester Di(2-ethylhexyl) fumarate Fumaric acid, di(2-ethylhexyl) ester 2-Butenedioic acid (E)-,di(2-ethylhexyl) ester 2-Butenedioic acid (2E)-, 1,4-bis(2-ethylhexyl) ester 2-Butenedioic acid (2E)-, bis(2-ethylhexyl) ester Dioctyl fumarate Bis(2-ethylhexyl) (2e)-2-butenedioate
Inchi:	InChI=1S/C20H36O4/c1-5-9-11-17(7-3)15-23-19(21)13-14-20(22)24-16-18(8-4)12-10-6-2
InchiKey:	ROPXFXOUUANXRR-BUHFOSPRSA-N
Formula:	C20H36O4
SMILES:	CCCCC(CC)COC(=O)C=CC(=O)OCC(CC)CCCC
Mol. weight [g/mol]:	340.50
CAS:	141-02-6

Physical Properties

Property code	Value	Unit	Source
gf	-274.98	kJ/mol	Joback Method
hf	-839.07	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	77.61	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	5.062		Crippen Method
mvol	303.240	ml/mol	McGowan Method
pc	1127.59	kPa	Joback Method
tb	812.86	K	Joback Method
tc	1000.99	K	Joback Method
tf	424.40	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.85	J/molxK	812.86	Joback Method
cpg	962.71	J/molxK	844.21	Joback Method
cpg	979.55	J/molxK	875.57	Joback Method
cpg	995.38	J/molxK	906.92	Joback Method
cpg	1010.22	J/molxK	938.28	Joback Method
cpg	1024.11	J/molxK	969.63	Joback Method
cpg	1037.07	J/molxK	1000.99	Joback Method
dvisc	0.0011216	Paxs	424.40	Joback Method
dvisc	0.0004425	Paxs	489.14	Joback Method
dvisc	0.0002170	Paxs	553.89	Joback Method
dvisc	0.0001235	Paxs	618.63	Joback Method
dvisc	0.0000782	Paxs	683.37	Joback Method
dvisc	0.0000536	Paxs	748.12	Joback Method
dvisc	0.0000390	Paxs	812.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141026&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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