2-Butenedioic acid (E)-, dibutyl ester

Other names:	Fumaric acid, dibutyl ester
	Butyl fumarate
	Dibutyl fumarate
	RC Comonomer DBF
	Staflex DBF
	Dibutylester kyseliny fumarove
	Dibutyl ester of fumaric acid
	Di-n-butyl fumarate
	Bisomer DBF
	2-Butenedioic acid (2E)-, 1,4-dibutyl ester
	2-Butenedioic acid (2E)-, dibutyl ester
	NSC 140
	Dibutyl (2e)-2-butenedioate
Inchi:	InChI=1S/C12H20O4/c1-3-5-9-15-11(13)7-8-12(14)16-10-6-4-2/h7-8H,3-6,9-10H2,1-2H3
InchiKey:	JBSLOWBPDRZSMB-BQYQJAHWSA-N
Formula:	C12H20O4
SMILES:	CCCCOC(=O)C=CC(=O)OCCCC
Mol. weight [g/mol]:	228.28
CAS:	105-75-9

Physical Properties

Property code	Value	Unit	Source
gf	-337.46	kJ/mol	Joback Method
hf	-663.39	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	60.58	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.229		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	1558.00		NIST Webbook
rinpol	1556.00		NIST Webbook
tb	630.70	K	Joback Method
tc	814.25	K	Joback Method
tf	255.25 ± 0.20	K	NIST Webbook
tf	254.95 ± 0.30	K	NIST Webbook
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.03	J/mol×K	630.70	Joback Method
cpg	509.10	J/mol×K	661.29	Joback Method
cpg	522.51	J/mol×K	691.88	Joback Method
cpg	535.27	J/mol×K	722.48	Joback Method
cpg	547.40	J/mol×K	753.07	Joback Method
cpg	558.89	J/mol×K	783.66	Joback Method
cpg	569.75	J/mol×K	814.25	Joback Method
dvisc	0.0015837	Pa×s	364.24	Joback Method
dvisc	0.0008330	Pa×s	408.65	Joback Method
dvisc	0.0004970	Pa×s	453.06	Joback Method
dvisc	0.0003252	Pa×s	497.47	Joback Method
dvisc	0.0002281	Pa×s	541.88	Joback Method
dvisc	0.0001688	Pa×s	586.29	Joback Method
dvisc	0.0001303	Pa×s	630.70	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=C105759&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
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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