

Fumaric acid, butyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C14H22O4/c1-3-5-7-8-12-18-14(16)10-9-13(15)17-11-6-4-2/h5,7,9-10H,3-4,6,8
InchiKey:	ZXNHJMOLFCNSCY-GLVZAGOZSA-N
Formula:	C14H22O4
SMILES:	CCC=CCCOC(=O)C=CC(=O)OCCCC
Mol. weight [g/mol]:	254.32

Physical Properties

Property code	Value	Unit	Source
gf	-240.40	kJ/mol	Joback Method
hf	-587.45	kJ/mol	Joback Method
hfus	37.99	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.785		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinqol	1779.00		NIST Webbook
tb	680.62	K	Joback Method
tc	867.57	K	Joback Method
tf	381.70	K	Joback Method
vc	0.828	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.81	J/molxK	680.62	Joback Method
cpg	592.46	J/molxK	711.78	Joback Method
cpg	606.36	J/molxK	742.94	Joback Method
cpg	619.54	J/molxK	774.09	Joback Method
cpg	632.01	J/molxK	805.25	Joback Method
cpg	643.81	J/molxK	836.41	Joback Method
cpg	654.95	J/molxK	867.57	Joback Method
dvisc	0.0012769	Paxs	381.70	Joback Method
dvisc	0.0006335	Paxs	431.52	Joback Method

dvisc	0.0003633	Paxs	481.34	Joback Method
dvisc	0.0002313	Paxs	531.16	Joback Method
dvisc	0.0001591	Paxs	580.98	Joback Method
dvisc	0.0001161	Paxs	630.80	Joback Method
dvisc	0.0000887	Paxs	680.62	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=U348885&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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