Fumaric acid, butyl cis-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-ROBNAOGRSA-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
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	680.62	K	Joback Method
tc	867.57	K	Joback Method
tf	381.70	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.81	J/mol×K	680.62	Joback Method
cpg	592.46	J/mol×K	711.78	Joback Method
cpg	606.36	J/mol×K	742.94	Joback Method
cpg	619.54	J/mol×K	774.09	Joback Method
cpg	632.01	J/mol×K	805.25	Joback Method
cpg	643.81	J/mol×K	836.41	Joback Method
cpg	654.95	J/mol×K	867.57	Joback Method
dvisc	0.0012769	Pa×s	381.70	Joback Method

dvisc	0.0006335	Pa×s	431.52	Joback Method
dvisc	0.0003633	Pa×s	481.34	Joback Method
dvisc	0.0002313	Pa×s	531.16	Joback Method
dvisc	0.0001591	Pa×s	580.98	Joback Method
dvisc	0.0001161	Pa×s	630.80	Joback Method
dvisc	0.0000887	Pa×s	680.62	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U348861&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