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

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

Physical Properties

Property code	Value	Unit	Source
gf	-242.84	kJ/mol	Joback Method
hf	-592.73	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.641		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
tb	680.18	K	Joback Method
tc	869.98	K	Joback Method
tf	366.70	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.30	J/mol×K	680.18	Joback Method
cpg	645.26	J/mol×K	838.34	Joback Method
cpg	633.33	J/mol×K	806.71	Joback Method
cpg	620.69	J/mol×K	775.08	Joback Method
cpg	607.33	J/mol×K	743.45	Joback Method
cpg	593.20	J/mol×K	711.81	Joback Method
cpg	656.50	J/mol×K	869.98	Joback Method
dvisc	0.0000822	Pa×s	680.18	Joback Method

dvisc	0.0001097	Pa×s	627.93	Joback Method
dvisc	0.0001541	Pa×s	575.69	Joback Method
dvisc	0.0002319	Pa×s	523.44	Joback Method
dvisc	0.0003819	Pa×s	471.19	Joback Method
dvisc	0.0007124	Pa×s	418.95	Joback Method
dvisc	0.0015872	Pa×s	366.70	Joback Method

Sources

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=U348884&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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