Fumaric acid, hexyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C14H22O5/c1-4-5-6-7-10-18-13(16)8-9-14(17)19-12(3)11(2)15/h8-9,12H,4-7,1
InchiKey: ZHRFVSDJOSIEJI-CMDGGOBGSA-N
Formula: C14H22O5
SMILES: CCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 270.32

Physical Properties

Property code	Value	Unit	Source
gf	-451.98	kJ/mol	Joback Method
hf	-822.53	kJ/mol	Joback Method
hfus	35.87	kJ/mol	Joback Method
hvap	71.39	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.187		Crippen Method
mcvol	220.270	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	1861.00		NIST Webbook
tb	729.89	K	Joback Method
tc	921.00	K	Joback Method
tf	421.71	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.53	J/mol×K	729.89	Joback Method
cpg	634.65	J/mol×K	761.74	Joback Method
cpg	647.97	J/mol×K	793.59	Joback Method
cpg	660.49	J/mol×K	825.44	Joback Method
cpg	672.24	J/mol×K	857.29	Joback Method
cpg	683.21	J/mol×K	889.14	Joback Method
cpg	693.43	J/mol×K	921.00	Joback Method
dvisc	0.0012972	Pa×s	421.71	Joback Method
dvisc	0.0006598	Pa×s	473.07	Joback Method

dvisc	0.0003832	Pa×s	524.44	Joback Method
dvisc	0.0002451	Pa×s	575.80	Joback Method
dvisc	0.0001688	Pa×s	627.16	Joback Method
dvisc	0.0001229	Pa×s	678.53	Joback Method
dvisc	0.0000936	Pa×s	729.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348820&Units=SI
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

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