Fumaric acid, 3-methylbut-2-yl pentyl ester

Inchi: InChI=1S/C14H24O4/c1-5-6-7-10-17-13(15)8-9-14(16)18-12(4)11(2)3/h8-9,11-12H,5-7,1
InchiKey: YGSZSBLSSQIVRK-CMDGGOBGSA-N
Formula: C14H24O4
SMILES: CCCCCOC(=O)C=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-325.50	kJ/mol	Joback Method
hf	-715.23	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	64.25	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.864		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1689.00		NIST Webbook
tb	675.58	K	Joback Method
tc	862.18	K	Joback Method
tf	356.78	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.07	J/mol×K	675.58	Joback Method
cpg	616.74	J/mol×K	706.68	Joback Method
cpg	631.60	J/mol×K	737.78	Joback Method
cpg	645.68	J/mol×K	768.88	Joback Method
cpg	658.99	J/mol×K	799.98	Joback Method
cpg	671.55	J/mol×K	831.08	Joback Method
cpg	683.37	J/mol×K	862.18	Joback Method
dvisc	0.0021664	Pa×s	356.78	Joback Method
dvisc	0.0009003	Pa×s	409.91	Joback Method

dvisc	0.0004576	Pa×s	463.05	Joback Method
dvisc	0.0002674	Pa×s	516.18	Joback Method
dvisc	0.0001727	Pa×s	569.31	Joback Method
dvisc	0.0001202	Pa×s	622.45	Joback Method
dvisc	0.0000886	Pa×s	675.58	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=U348077&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