Fumaric acid, 3,3-dimethylbut-2-yl propyl ester

Inchi: InChI=1S/C13H22O4/c1-6-9-16-11(14)7-8-12(15)17-10(2)13(3,4)5/h7-8,10H,6,9H2,1-5H
InchiKey: OWDRQADJYYYCLG-BQYQJAHWSA-N
Formula: C13H22O4
SMILES: CCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-328.64	kJ/mol	Joback Method
hf	-698.06	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	61.12	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.474		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1537.00		NIST Webbook
rinpol	1537.00		NIST Webbook
tb	649.91	K	Joback Method
tc	843.73	K	Joback Method
tf	362.93	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.22	J/mol×K	649.91	Joback Method
cpg	565.66	J/mol×K	682.21	Joback Method
cpg	580.25	J/mol×K	714.52	Joback Method
cpg	594.01	J/mol×K	746.82	Joback Method
cpg	606.98	J/mol×K	779.12	Joback Method
cpg	619.18	J/mol×K	811.43	Joback Method
cpg	630.63	J/mol×K	843.73	Joback Method
dvisc	0.0020140	Pa×s	362.93	Joback Method

dvisc	0.0008956	Pa×s	410.76	Joback Method
dvisc	0.0004717	Pa×s	458.59	Joback Method
dvisc	0.0002804	Pa×s	506.42	Joback Method
dvisc	0.0001823	Pa×s	554.25	Joback Method
dvisc	0.0001269	Pa×s	602.08	Joback Method
dvisc	0.0000932	Pa×s	649.91	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=U348700&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