Fumaric acid, 2,4-dimethylpent-3-yl ethyl ester

Inchi: InChI=1S/C13H22O4/c1-6-16-11(14)7-8-12(15)17-13(9(2)3)10(4)5/h7-10,13H,6H2,1-5H3
InchiKey: DYBLWEWBQMIHGS-BQYQJAHWSA-N
Formula: C13H22O4
SMILES: CCOC(=O)C=CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-336.36	kJ/mol	Joback Method
hf	-699.87	kJ/mol	Joback Method
hfus	24.63	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.329		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1528.00		NIST Webbook
rinpol	1528.00		NIST Webbook
tb	652.26	K	Joback Method
tc	843.44	K	Joback Method
tf	330.51	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.27	J/mol×K	652.26	Joback Method
cpg	563.73	J/mol×K	684.12	Joback Method
cpg	578.41	J/mol×K	715.99	Joback Method
cpg	592.30	J/mol×K	747.85	Joback Method
cpg	605.43	J/mol×K	779.71	Joback Method
cpg	617.79	J/mol×K	811.58	Joback Method
cpg	629.41	J/mol×K	843.44	Joback Method
dvisc	0.0031577	Pa×s	330.51	Joback Method

dvisc	0.0011650	Pa×s	384.13	Joback Method
dvisc	0.0005487	Pa×s	437.76	Joback Method
dvisc	0.0003046	Pa×s	491.38	Joback Method
dvisc	0.0001899	Pa×s	545.01	Joback Method
dvisc	0.0001288	Pa×s	598.63	Joback Method
dvisc	0.0000931	Pa×s	652.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348541&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

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

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