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

Inchi: InChI=1S/C12H20O4/c1-6-15-10(13)7-8-11(14)16-9(2)12(3,4)5/h7-9H,6H2,1-5H3/b8-7+
InchiKey: FGMPNDDYAKNOAP-BQYQJAHWSA-N
Formula: C12H20O4
SMILES: CCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 228.28

Physical Properties

Property code	Value	Unit	Source
gf	-337.06	kJ/mol	Joback Method
hf	-677.42	kJ/mol	Joback Method
hfus	21.68	kJ/mol	Joback Method
hvap	58.89	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.083		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1449.00		NIST Webbook
tb	627.03	K	Joback Method
tc	823.12	K	Joback Method
tf	351.66	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.56	J/mol×K	627.03	Joback Method
cpg	513.50	J/mol×K	659.71	Joback Method
cpg	527.61	J/mol×K	692.39	Joback Method
cpg	540.92	J/mol×K	725.08	Joback Method
cpg	553.47	J/mol×K	757.76	Joback Method
cpg	565.26	J/mol×K	790.44	Joback Method
cpg	576.34	J/mol×K	823.12	Joback Method
dvisc	0.0022139	Pa×s	351.66	Joback Method
dvisc	0.0009966	Pa×s	397.55	Joback Method

dvisc	0.0005292	Pa×s	443.45	Joback Method
dvisc	0.0003164	Pa×s	489.34	Joback Method
dvisc	0.0002066	Pa×s	535.24	Joback Method
dvisc	0.0001443	Pa×s	581.13	Joback Method
dvisc	0.0001063	Pa×s	627.03	Joback Method

Sources

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=U348699&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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