Fumaric acid, ethyl 2-ethylbutyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-339.90	kJ/mol	Joback Method
hf	-668.67	kJ/mol	Joback Method
hfus	29.09	kJ/mol	Joback Method
hvap	60.19	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.085		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	1542.00		NIST Webbook
tb	630.26	K	Joback Method
tc	816.90	K	Joback Method
tf	349.24	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.48	J/mol×K	630.26	Joback Method
cpg	509.82	J/mol×K	661.37	Joback Method
cpg	523.48	J/mol×K	692.47	Joback Method
cpg	536.46	J/mol×K	723.58	Joback Method
cpg	548.77	J/mol×K	754.69	Joback Method
cpg	560.42	J/mol×K	785.80	Joback Method
cpg	571.41	J/mol×K	816.90	Joback Method
dvisc	0.0019896	Pa×s	349.24	Joback Method
dvisc	0.0009475	Pa×s	396.08	Joback Method

dvisc	0.0005279	Pa×s	442.91	Joback Method
dvisc	0.0003289	Pa×s	489.75	Joback Method
dvisc	0.0002226	Pa×s	536.59	Joback Method
dvisc	0.0001604	Pa×s	583.42	Joback Method
dvisc	0.0001213	Pa×s	630.26	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=U405644&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

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