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

Inchi: InChI=1S/C11H18O4/c1-5-14-10(12)6-7-11(13)15-9(4)8(2)3/h6-9H,5H2,1-4H3/b7-6+
InchiKey: ZYMNTZKXROHRFD-VOTSOKGWSA-N
Formula: C11H18O4
SMILES: CCOC(=O)C=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
gf	-350.76	kJ/mol	Joback Method
hf	-653.31	kJ/mol	Joback Method
hfus	22.98	kJ/mol	Joback Method
hvap	57.57	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.693		Crippen Method
mcvol	176.430	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1384.00		NIST Webbook
tb	606.94	K	Joback Method
tc	798.94	K	Joback Method
tf	322.97	K	Joback Method
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.51	J/mol×K	606.94	Joback Method
cpg	508.86	J/mol×K	766.94	Joback Method
cpg	497.52	J/mol×K	734.94	Joback Method
cpg	485.52	J/mol×K	702.94	Joback Method
cpg	472.86	J/mol×K	670.94	Joback Method
cpg	459.53	J/mol×K	638.94	Joback Method
cpg	519.56	J/mol×K	798.94	Joback Method
dvisc	0.0001266	Pa×s	606.94	Joback Method
dvisc	0.0001704	Pa×s	559.61	Joback Method

dvisc	0.0002424	Pa×s	512.28	Joback Method
dvisc	0.0003705	Pa×s	464.95	Joback Method
dvisc	0.0006233	Pa×s	417.63	Joback Method
dvisc	0.0011979	Pa×s	370.30	Joback Method
dvisc	0.0027881	Pa×s	322.97	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=U348074&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