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

Inchi: InChI=1S/C14H24O4/c1-10(2)8-9-17-13(15)6-7-14(16)18-12(5)11(3)4/h6-7,10-12H,8-9H
InchiKey: SUKUBDSKMDHWTI-VOTSOKGWSA-N
Formula: C14H24O4
SMILES: CC(C)CCOC(=O)C=CC(=O)OC(C)C(C)C
Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-327.94	kJ/mol	Joback Method
hf	-720.51	kJ/mol	Joback Method
hfus	27.22	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.720		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tb	675.14	K	Joback Method
tc	864.61	K	Joback Method
tf	341.78	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.55	J/mol×K	675.14	Joback Method
cpg	673.06	J/mol×K	833.03	Joback Method
cpg	660.36	J/mol×K	801.46	Joback Method
cpg	646.87	J/mol×K	769.88	Joback Method
cpg	632.58	J/mol×K	738.30	Joback Method
cpg	617.48	J/mol×K	706.72	Joback Method
cpg	684.98	J/mol×K	864.61	Joback Method
dvisc	0.0000821	Pa×s	675.14	Joback Method

dvisc	0.0001138	Pa×s	619.58	Joback Method
dvisc	0.0001681	Pa×s	564.02	Joback Method
dvisc	0.0002705	Pa×s	508.46	Joback Method
dvisc	0.0004891	Pa×s	452.90	Joback Method
dvisc	0.0010436	Pa×s	397.34	Joback Method
dvisc	0.0028493	Pa×s	341.78	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=U405548&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