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

Inchi: InChI=1S/C14H24O4/c1-6-7-10-17-12(15)8-9-13(16)18-11(2)14(3,4)5/h8-9,11H,6-7,10H2
InchiKey: CQZZIOVGONTWTC-CMDGGOBGSA-N
Formula: C14H24O4
SMILES: CCCCOC(=O)C=CC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-320.22	kJ/mol	Joback Method
hf	-718.70	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	63.34	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.864		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
tb	672.79	K	Joback Method
tc	864.68	K	Joback Method
tf	374.20	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.25	J/mol×K	672.79	Joback Method
cpg	674.15	J/mol×K	832.70	Joback Method
cpg	661.60	J/mol×K	800.72	Joback Method
cpg	648.27	J/mol×K	768.74	Joback Method
cpg	634.12	J/mol×K	736.75	Joback Method
cpg	619.12	J/mol×K	704.77	Joback Method
cpg	685.94	J/mol×K	864.68	Joback Method
dvisc	0.0000815	Pa×s	672.79	Joback Method

dvisc	0.0001112	Pa×s	623.02	Joback Method
dvisc	0.0001601	Pa×s	573.26	Joback Method
dvisc	0.0002473	Pa×s	523.50	Joback Method
dvisc	0.0004183	Pa×s	473.73	Joback Method
dvisc	0.0008006	Pa×s	423.97	Joback Method
dvisc	0.0018211	Pa×s	374.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348702&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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