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

Inchi: InChI=1S/C12H18O5/c1-4-5-8-16-11(14)6-7-12(15)17-10(3)9(2)13/h6-7,10H,4-5,8H2,1-3
InchiKey: NINYMJGCDLFJIG-VOTSOKGWSA-N
Formula: C12H18O5
SMILES: CCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 242.27

Physical Properties

Property code	Value	Unit	Source
gf	-468.82	kJ/mol	Joback Method
hf	-781.25	kJ/mol	Joback Method
hfus	30.69	kJ/mol	Joback Method
hvap	66.93	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.407		Crippen Method
mcvol	192.090	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1659.00		NIST Webbook
tb	684.13	K	Joback Method
tc	877.89	K	Joback Method
tf	399.17	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.95	J/mol×K	684.13	Joback Method
cpg	572.57	J/mol×K	845.60	Joback Method
cpg	562.27	J/mol×K	813.31	Joback Method
cpg	551.26	J/mol×K	781.01	Joback Method
cpg	539.54	J/mol×K	748.72	Joback Method
cpg	527.11	J/mol×K	716.42	Joback Method
cpg	582.19	J/mol×K	877.89	Joback Method
dvisc	0.0001207	Pa×s	684.13	Joback Method
dvisc	0.0001574	Pa×s	636.64	Joback Method

dvisc	0.0002143	Pa×s	589.14	Joback Method
dvisc	0.0003080	Pa×s	541.65	Joback Method
dvisc	0.0004746	Pa×s	494.16	Joback Method
dvisc	0.0008019	Pa×s	446.66	Joback Method
dvisc	0.0015348	Pa×s	399.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348819&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