Fumaric acid, butyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C13H20O4/c1-4-5-9-16-12(14)6-7-13(15)17-10-8-11(2)3/h6-7H,2,4-5,8-10H2,1
InchiKey: CDLNIKGMZNTHKD-VOTSOKGWSA-N
Formula: C13H20O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCC
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	-249.75	kJ/mol	Joback Method
hf	-568.39	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	62.21	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.395		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1932.13	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
tb	650.14	K	Joback Method
tc	837.55	K	Joback Method
tf	359.79	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.05	J/mol×K	650.14	Joback Method
cpg	538.30	J/mol×K	681.37	Joback Method
cpg	551.84	J/mol×K	712.61	Joback Method
cpg	564.69	J/mol×K	743.84	Joback Method
cpg	576.85	J/mol×K	775.08	Joback Method
cpg	588.35	J/mol×K	806.31	Joback Method
cpg	599.19	J/mol×K	837.55	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=U348902&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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