Fumaric acid, isobutyl myrtenyl ester

Inchi: InChI=1S/C18H26O4/c1-12(2)10-21-16(19)5-6-17(20)22-11-13-7-14-9-15(8-13)18(14,3)4
InchiKey: ZNIKRHJVVJVRBN-AATRIKPKSA-N
Formula: C18H26O4
SMILES: CC(C)COC(=O)C=CC(=O)OCC1=CC2CC(C1)C2(C)C
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-172.85	kJ/mol	Joback Method
hf	-611.86	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	73.04	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.277		Crippen Method
mcvol	249.040	ml/mol	McGowan Method
pc	1631.17	kPa	Joback Method
rinpol	2093.00		NIST Webbook
tb	785.00	K	Joback Method
tc	994.36	K	Joback Method
tf	482.16	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.41	J/mol×K	785.00	Joback Method
cpg	787.42	J/mol×K	819.89	Joback Method
cpg	804.82	J/mol×K	854.79	Joback Method
cpg	821.77	J/mol×K	889.68	Joback Method
cpg	838.39	J/mol×K	924.58	Joback Method
cpg	854.83	J/mol×K	959.47	Joback Method
cpg	871.21	J/mol×K	994.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348811&Units=SI

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