Fumaric acid, myrtenyl propyl ester

Inchi: InChI=1S/C17H24O4/c1-4-7-20-15(18)5-6-16(19)21-11-12-8-13-10-14(9-12)17(13,2)3/h5
InchiKey: VYODHYVKJAQTRZ-AATRIKPKSA-N
Formula: C17H24O4
SMILES: CCCOC(=O)C=CC(=O)OCC1=CC2CC(C1)C2(C)C
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	-178.83	kJ/mol	Joback Method
hf	-585.94	kJ/mol	Joback Method
hfus	35.34	kJ/mol	Joback Method
hvap	71.20	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.031		Crippen Method
mcvol	234.950	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	2039.00		NIST Webbook
tb	762.56	K	Joback Method
tc	970.82	K	Joback Method
tf	485.89	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.52	J/mol×K	762.56	Joback Method
cpg	728.79	J/mol×K	797.27	Joback Method
cpg	745.44	J/mol×K	831.98	Joback Method
cpg	761.62	J/mol×K	866.69	Joback Method
cpg	777.46	J/mol×K	901.40	Joback Method
cpg	793.08	J/mol×K	936.11	Joback Method
cpg	808.63	J/mol×K	970.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348810&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
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