Fumaric acid, hexyl myrtenyl ester

Inchi: InChI=1S/C20H30O4/c1-4-5-6-7-10-23-18(21)8-9-19(22)24-14-15-11-16-13-17(12-15)20
InchiKey: QYQZUXPYFDWJAY-CMDGGOBGSA-N
Formula: C20H30O4
SMILES: CCCCCCOC(=O)C=CC(=O)OCC1=CC2CC(C1)C2(C)C
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-153.57	kJ/mol	Joback Method
hf	-647.86	kJ/mol	Joback Method
hfus	43.11	kJ/mol	Joback Method
hvap	77.88	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.202		Crippen Method
mcvol	277.220	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	2354.00		NIST Webbook
tb	831.20	K	Joback Method
tc	1035.98	K	Joback Method
tf	519.70	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.98	J/mol×K	831.20	Joback Method
cpg	905.81	J/mol×K	865.33	Joback Method
cpg	924.14	J/mol×K	899.46	Joback Method
cpg	942.10	J/mol×K	933.59	Joback Method
cpg	959.83	J/mol×K	967.72	Joback Method
cpg	977.46	J/mol×K	1001.85	Joback Method
cpg	995.13	J/mol×K	1035.98	Joback Method

Sources

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=U348815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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