Fumaric acid, myrtenyl pentyl ester

Inchi: InChI=1S/C19H28O4/c1-4-5-6-9-22-17(20)7-8-18(21)23-13-14-10-15-12-16(11-14)19(15
InchiKey: YSLLUVNGWBKQTK-BQYQJAHWSA-N
Formula: C19H28O4
SMILES: CCCCCOC(=O)C=CC(=O)OCC1=CC2CC(C1)C2(C)C
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-161.99	kJ/mol	Joback Method
hf	-627.22	kJ/mol	Joback Method
hfus	40.52	kJ/mol	Joback Method
hvap	75.65	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.812		Crippen Method
mcvol	263.130	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2243.00		NIST Webbook
tb	808.32	K	Joback Method
tc	1013.66	K	Joback Method
tf	508.43	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.39	J/mol×K	808.32	Joback Method
cpg	845.67	J/mol×K	842.54	Joback Method
cpg	863.42	J/mol×K	876.77	Joback Method
cpg	880.76	J/mol×K	910.99	Joback Method
cpg	897.82	J/mol×K	945.21	Joback Method
cpg	914.75	J/mol×K	979.43	Joback Method
cpg	931.68	J/mol×K	1013.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348813&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