Fumaric acid, myrtenyl octyl ester

Inchi: InChI=1S/C22H34O4/c1-4-5-6-7-8-9-12-25-20(23)10-11-21(24)26-16-17-13-18-15-19(14
InchiKey: QQQLDTKPIVKDDD-ZHACJKMWSA-N
Formula: C22H34O4
SMILES: CCCCCCCCOC(=O)C=CC(=O)OCC1=CC2CC(C1)C2(C)C
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-136.73	kJ/mol	Joback Method
hf	-689.14	kJ/mol	Joback Method
hfus	48.29	kJ/mol	Joback Method
hvap	82.33	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.982		Crippen Method
mcvol	305.400	ml/mol	McGowan Method
pc	1215.74	kPa	Joback Method
rinpol	2565.00		NIST Webbook
tb	876.96	K	Joback Method
tc	1082.67	K	Joback Method
tf	542.24	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.29	J/mol×K	876.96	Joback Method
cpg	1029.36	J/mol×K	911.24	Joback Method
cpg	1049.00	J/mol×K	945.53	Joback Method
cpg	1068.36	J/mol×K	979.81	Joback Method
cpg	1087.58	J/mol×K	1014.10	Joback Method
cpg	1106.80	J/mol×K	1048.38	Joback Method
cpg	1126.17	J/mol×K	1082.67	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=U348817&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