Fumaric acid, dimyrtenyl ester

Inchi: InChI=1S/C24H32O4/c1-23(2)17-7-15(8-18(23)11-17)13-27-21(25)5-6-22(26)28-14-16-9
InchiKey: PZZSDJFWIZUMDC-AATRIKPKSA-N
Formula: C24H32O4
SMILES: CC1(C)C2C=C(COC(=O)C=CC(=O)OCC3=CC4CC(C3)C4(C)C)CC1C2
Mol. weight [g/mol]: 384.51

Physical Properties

Property code	Value	Unit	Source
gf	-3.36	kJ/mol	Joback Method
hf	-549.77	kJ/mol	Joback Method
hfus	43.24	kJ/mol	Joback Method
hvap	86.27	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.614		Crippen Method
mcvol	307.560	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	2746.00		NIST Webbook
tb	940.18	K	Joback Method
tc	1168.58	K	Joback Method
tf	630.08	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1082.11	J/mol×K	940.18	Joback Method
cpg	1108.36	J/mol×K	978.25	Joback Method
cpg	1135.57	J/mol×K	1016.31	Joback Method
cpg	1164.09	J/mol×K	1054.38	Joback Method
cpg	1194.26	J/mol×K	1092.44	Joback Method
cpg	1226.41	J/mol×K	1130.51	Joback Method
cpg	1260.89	J/mol×K	1168.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348818&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