Fumaric acid, heptyl myrtenyl ester

Inchi: InChI=1S/C21H32O4/c1-4-5-6-7-8-11-24-19(22)9-10-20(23)25-15-16-12-17-14-18(13-16
InchiKey: BONXKMQLOFUNQF-MDZDMXLPSA-N
Formula: C21H32O4
SMILES: CCCCCCCOC(=O)C=CC(=O)OCC1=CC2CC(C1)C2(C)C
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-145.15	kJ/mol	Joback Method
hf	-668.50	kJ/mol	Joback Method
hfus	45.70	kJ/mol	Joback Method
hvap	80.10	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.592		Crippen Method
mcvol	291.310	ml/mol	McGowan Method
pc	1301.41	kPa	Joback Method
rinpol	2459.00		NIST Webbook
rinpol	2459.00		NIST Webbook
tb	854.08	K	Joback Method
tc	1058.96	K	Joback Method
tf	530.97	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.63	J/mol×K	854.08	Joback Method
cpg	967.05	J/mol×K	888.23	Joback Method
cpg	986.00	J/mol×K	922.37	Joback Method
cpg	1004.63	J/mol×K	956.52	Joback Method
cpg	1023.07	J/mol×K	990.67	Joback Method
cpg	1041.46	J/mol×K	1024.82	Joback Method
cpg	1059.94	J/mol×K	1058.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348816&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