Fumaric acid, butyl myrtenyl ester

Inchi: InChI=1S/C18H26O4/c1-4-5-8-21-16(19)6-7-17(20)22-12-13-9-14-11-15(10-13)18(14,2)3
InchiKey: FGLVSEZGGYEAAD-VOTSOKGWSA-N
Formula: C18H26O4
SMILES: CCCCOC(=O)C=CC(=O)OCC1=CC2CC(C1)C2(C)C
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-170.41	kJ/mol	Joback Method
hf	-606.58	kJ/mol	Joback Method
hfus	37.93	kJ/mol	Joback Method
hvap	73.42	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.421		Crippen Method
mcvol	249.040	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	2140.00		NIST Webbook
rinpol	2140.00		NIST Webbook
tb	785.44	K	Joback Method
tc	991.95	K	Joback Method
tf	497.16	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.89	J/mol×K	785.44	Joback Method
cpg	786.66	J/mol×K	819.86	Joback Method
cpg	803.85	J/mol×K	854.28	Joback Method
cpg	820.60	J/mol×K	888.70	Joback Method
cpg	837.04	J/mol×K	923.12	Joback Method
cpg	853.30	J/mol×K	957.54	Joback Method
cpg	869.52	J/mol×K	991.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348812&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

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