Fumaric acid, 3-phenylpropyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C16H17F3O4/c1-12(16(17,18)19)23-15(21)10-9-14(20)22-11-5-8-13-6-3-2-4-7

InchiKey: GNTNPFWTCQLNFZ-MDZDMXLPSA-N

Formula: C16H17F3O4

SMILES: CC(OC(=O)C=CC(=O)OCCCc1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 330.30

Physical Properties

Property code	Value	Unit	Source
gf	-775.40	kJ/mol	Joback Method
hf	-1111.78	kJ/mol	Joback Method
hfus	35.32	kJ/mol	Joback Method
hvap	67.62	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.213		Crippen Method
mcvol	228.430	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1854.00		NIST Webbook
rinpol	1854.00		NIST Webbook
tb	743.04	K	Joback Method
tc	940.90	K	Joback Method
tf	424.93	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.97	J/mol×K	743.04	Joback Method
cpg	664.50	J/mol×K	776.02	Joback Method
cpg	677.10	J/mol×K	808.99	Joback Method
cpg	688.80	J/mol×K	841.97	Joback Method
cpg	699.66	J/mol×K	874.95	Joback Method
cpg	709.71	J/mol×K	907.92	Joback Method
cpg	719.01	J/mol×K	940.90	Joback Method

Sources

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=U405658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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