Fumaric acid, 1-phenylprop-1-yl 1,1,1-trifluoroprop-2-yl ester

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

InchiKey: BVAROYDOEYVFSP-MDZDMXLPSA-N

Formula: C16H17F3O4

SMILES: CCC(OC(=O)C=CC(=O)OC(C)C(F)(F)F)c1ccccc1

Mol. weight [g/mol]: 330.30

Physical Properties

Property code	Value	Unit	Source
gf	-777.84	kJ/mol	Joback Method
hf	-1117.06	kJ/mol	Joback Method
hfus	31.79	kJ/mol	Joback Method
hvap	67.23	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.731		Crippen Method
mcvol	228.430	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
tb	742.60	K	Joback Method
tc	943.28	K	Joback Method
tf	409.93	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.53	J/mol×K	742.60	Joback Method
cpg	665.27	J/mol×K	776.05	Joback Method
cpg	678.03	J/mol×K	809.49	Joback Method
cpg	689.87	J/mol×K	842.94	Joback Method
cpg	700.82	J/mol×K	876.38	Joback Method
cpg	710.95	J/mol×K	909.83	Joback Method
cpg	720.29	J/mol×K	943.28	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=U405896&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