Fumaric acid, 3-phenylpropyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C16H16F4O4/c17-15(18)16(19,20)11-24-14(22)9-8-13(21)23-10-4-7-12-5-2-1-

InchiKey: JUOQLNCRPQMAQB-CMDGGOBGSA-N

Formula: C16H16F4O4

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

Mol. weight [g/mol]: 348.29

Physical Properties

Property code	Value	Unit	Source
gf	-970.21	kJ/mol	Joback Method
hf	-1307.89	kJ/mol	Joback Method
hfus	38.40	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.162		Crippen Method
mcvol	230.200	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	1945.00		NIST Webbook
tb	742.31	K	Joback Method
tc	934.08	K	Joback Method
tf	425.52	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.75	J/mol×K	742.31	Joback Method
cpg	671.79	J/mol×K	774.27	Joback Method
cpg	683.94	J/mol×K	806.23	Joback Method
cpg	695.25	J/mol×K	838.20	Joback Method
cpg	705.75	J/mol×K	870.16	Joback Method
cpg	715.48	J/mol×K	902.12	Joback Method
cpg	724.50	J/mol×K	934.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405659&Units=SI

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