Fumaric acid, 1-phenylprop-1-yl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C16H16F4O4/c1-2-12(11-6-4-3-5-7-11)24-14(22)9-8-13(21)23-10-16(19,20)15

InchiKey: ADBLNBOZOCGPEU-CMDGGOBGSA-N

Formula: C16H16F4O4

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

Mol. weight [g/mol]: 348.29

Physical Properties

Property code	Value	Unit	Source
gf	-972.65	kJ/mol	Joback Method
hf	-1313.17	kJ/mol	Joback Method
hfus	34.87	kJ/mol	Joback Method
hvap	66.42	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.681		Crippen Method
mcvol	230.200	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	1829.00		NIST Webbook
rinpol	1829.00		NIST Webbook
tb	741.87	K	Joback Method
tc	936.15	K	Joback Method
tf	410.52	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.31	J/mol×K	741.87	Joback Method
cpg	672.53	J/mol×K	774.25	Joback Method
cpg	684.84	J/mol×K	806.63	Joback Method
cpg	696.26	J/mol×K	839.01	Joback Method
cpg	706.85	J/mol×K	871.39	Joback Method
cpg	716.65	J/mol×K	903.77	Joback Method
cpg	725.70	J/mol×K	936.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405897&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