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

Inchi: InChI=1S/C15H14F4O4/c16-14(17)15(18,19)10-23-13(21)7-6-12(20)22-9-8-11-4-2-1-3-5

InchiKey: LZKLBSSFNBWEQO-VOTSOKGWSA-N

Formula: C15H14F4O4

SMILES: O=C(C=CC(=O)OCC(F)(F)C(F)F)OCCc1ccccc1

Mol. weight [g/mol]: 334.26

Physical Properties

Property code	Value	Unit	Source
gf	-978.63	kJ/mol	Joback Method
hf	-1287.25	kJ/mol	Joback Method
hfus	35.81	kJ/mol	Joback Method
hvap	64.58	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.772		Crippen Method
mcvol	216.110	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1831.00		NIST Webbook
rinpol	1831.00		NIST Webbook
tb	719.43	K	Joback Method
tc	912.15	K	Joback Method
tf	414.25	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.13	J/mol×K	719.43	Joback Method
cpg	617.80	J/mol×K	751.55	Joback Method
cpg	629.60	J/mol×K	783.67	Joback Method
cpg	640.56	J/mol×K	815.79	Joback Method
cpg	650.74	J/mol×K	847.91	Joback Method
cpg	660.16	J/mol×K	880.03	Joback Method
cpg	668.87	J/mol×K	912.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405676&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