3-phenylpropionyl glycine, PFP-TFE

Inchi: InChI=1S/C16H13F8NO4/c17-14(18,19)9-29-12(27)8-25(13(28)15(20,21)16(22,23)24)11
InchiKey: VZWHUPBRNBKZGR-UHFFFAOYSA-N
Formula: C16H13F8NO4
SMILES: O=C(CN(C(=O)CCc1ccccc1)C(=O)C(F)(F)C(F)(F)F)OCC(F)(F)F
Mol. weight [g/mol]: 435.27

Physical Properties

Property code	Value	Unit	Source
gf	-1734.69	kJ/mol	Joback Method
hf	-2134.60	kJ/mol	Joback Method
hfus	42.64	kJ/mol	Joback Method
hvap	67.75	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.278		Crippen Method
mcvol	247.260	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
tb	773.10	K	Joback Method
tc	957.07	K	Joback Method
tf	512.97	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.27	J/mol×K	773.10	Joback Method
cpg	757.31	J/mol×K	803.76	Joback Method
cpg	767.50	J/mol×K	834.42	Joback Method
cpg	776.90	J/mol×K	865.08	Joback Method
cpg	785.60	J/mol×K	895.74	Joback Method
cpg	793.65	J/mol×K	926.41	Joback Method
cpg	801.14	J/mol×K	957.07	Joback Method

Sources

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=R321685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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