Heptafluorobutyric acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C17H11F7O3/c18-15(19,16(20,21)17(22,23)24)14(25)27-13-8-6-12(7-9-13)26-

InchiKey: DANFPIMUIVVMHE-UHFFFAOYSA-N

Formula: C17H11F7O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 396.26

Physical Properties

Property code	Value	Unit	Source
gf	-1386.62	kJ/mol	Joback Method
hf	-1708.66	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	60.61	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.004		Crippen Method
mcvol	228.570	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1767.00		NIST Webbook
tb	730.61	K	Joback Method
tc	930.36	K	Joback Method
tf	452.49	K	Joback Method
vc	0.906	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.19	J/mol×K	730.61	Joback Method
cpg	672.76	J/mol×K	763.90	Joback Method
cpg	684.28	J/mol×K	797.19	Joback Method
cpg	694.82	J/mol×K	830.48	Joback Method
cpg	704.46	J/mol×K	863.78	Joback Method
cpg	713.28	J/mol×K	897.07	Joback Method
cpg	721.35	J/mol×K	930.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307632&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

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