Trifluoroacetic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C15H11F3O3/c16-15(17,18)14(19)21-13-8-6-12(7-9-13)20-10-11-4-2-1-3-5-11
InchiKey: VHEJEDRBSSNSAB-UHFFFAOYSA-N
Formula: C15H11F3O3
SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C(F)(F)F
Mol. weight [g/mol]: 296.24

Physical Properties

Property code	Value	Unit	Source
gf	-629.90	kJ/mol	Joback Method
hf	-865.44	kJ/mol	Joback Method
hfus	28.10	kJ/mol	Joback Method
hvap	62.02	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.733		Crippen Method
mcvol	193.310	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1700.00		NIST Webbook
tb	694.23	K	Joback Method
tc	911.73	K	Joback Method
tf	422.75	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.30	J/mol×K	694.23	Joback Method
cpg	531.83	J/mol×K	730.48	Joback Method
cpg	544.28	J/mol×K	766.73	Joback Method
cpg	555.70	J/mol×K	802.98	Joback Method
cpg	566.14	J/mol×K	839.23	Joback Method
cpg	575.65	J/mol×K	875.48	Joback Method
cpg	584.26	J/mol×K	911.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307658&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