2-Trifluoromethylbenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C21H15F3O3/c22-21(23,24)19-9-5-4-8-18(19)20(25)27-17-12-10-16(11-13-17)
InchiKey: YZYOOBLSNHOABH-UHFFFAOYSA-N
Formula: C21H15F3O3
SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 372.34

Physical Properties

Property code	Value	Unit	Source
gf	-476.60	kJ/mol	Joback Method
hf	-764.22	kJ/mol	Joback Method
hfus	37.29	kJ/mol	Joback Method
hvap	78.31	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.504		Crippen Method
mcvol	254.090	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook
tb	863.17	K	Joback Method
tc	1097.39	K	Joback Method
tf	529.31	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.82	J/mol×K	863.17	Joback Method
cpg	762.78	J/mol×K	902.21	Joback Method
cpg	774.45	J/mol×K	941.24	Joback Method
cpg	784.92	J/mol×K	980.28	Joback Method
cpg	794.28	J/mol×K	1019.32	Joback Method
cpg	802.60	J/mol×K	1058.35	Joback Method
cpg	809.98	J/mol×K	1097.39	Joback Method

Sources

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=U307675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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