2,5-Ditrifluoromethylbenzoic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C22H14F6O3/c23-21(24,25)15-6-11-19(22(26,27)28)18(12-15)20(29)31-17-9-7

InchiKey: MITDMBOEOCDKCI-UHFFFAOYSA-N

Formula: C22H14F6O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 440.34

Physical Properties

Property code	Value	Unit	Source
gf	-1059.40	kJ/mol	Joback Method
hf	-1393.41	kJ/mol	Joback Method
hfus	41.32	kJ/mol	Joback Method
hvap	77.45	kJ/mol	Joback Method
log10ws	-8.00		Crippen Method
logp	6.522		Crippen Method
mcvol	273.490	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2480.00		NIST Webbook
tb	885.61	K	Joback Method
tc	1106.36	K	Joback Method
tf	557.29	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.98	J/mol×K	885.61	Joback Method
cpg	839.73	J/mol×K	922.40	Joback Method
cpg	850.37	J/mol×K	959.19	Joback Method
cpg	860.02	J/mol×K	995.98	Joback Method
cpg	868.74	J/mol×K	1032.78	Joback Method
cpg	876.65	J/mol×K	1069.57	Joback Method
cpg	883.83	J/mol×K	1106.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357750&Units=SI

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