Phthalic acid, di(2-trifluorobenzyl) ester

Inchi: InChI=1S/C24H16F6O4/c25-23(26,27)19-11-5-1-7-15(19)13-33-21(31)17-9-3-4-10-18(17
InchiKey: HQZDVFVHGMRAOZ-UHFFFAOYSA-N
Formula: C24H16F6O4
SMILES: O=C(OCc1ccccc1C(F)(F)F)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 482.37

Physical Properties

Property code	Value	Unit	Source
gf	-1171.48	kJ/mol	Joback Method
hf	-1547.27	kJ/mol	Joback Method
hfus	48.10	kJ/mol	Joback Method
hvap	88.65	kJ/mol	Joback Method
log10ws	-8.38		Crippen Method
logp	6.438		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1357.63	kPa	Joback Method
rinpol	2675.00		NIST Webbook
rinpol	2675.00		NIST Webbook
tb	985.24	K	Joback Method
tc	1213.68	K	Joback Method
tf	629.76	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.10	J/mol×K	985.24	Joback Method
cpg	959.37	J/mol×K	1023.31	Joback Method
cpg	968.59	J/mol×K	1061.39	Joback Method
cpg	976.90	J/mol×K	1099.46	Joback Method
cpg	984.38	J/mol×K	1137.53	Joback Method
cpg	991.16	J/mol×K	1175.61	Joback Method
cpg	997.33	J/mol×K	1213.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377834&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