Phthalic acid, nonyl 2-trifluoromethylbenzyl ester

Other names: Phthalic acid, nonyl 2-trifluorobenzyl ester
Inchi: InChI=1S/C25H29F3O4/c1-2-3-4-5-6-7-12-17-31-23(29)20-14-9-10-15-21(20)24(30)32-1
InchiKey: WBGUUMYESCEYLN-UHFFFAOYSA-N
Formula: C25H29F3O4
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 450.49

Physical Properties

Property code	Value	Unit	Source
gf	-684.25	kJ/mol	Joback Method
hf	-1195.89	kJ/mol	Joback Method
hfus	55.21	kJ/mol	Joback Method
hvap	91.69	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	6.970		Crippen Method
mcvol	335.780	ml/mol	McGowan Method
pc	1103.74	kPa	Joback Method
rinpol	2809.00		NIST Webbook
tb	981.88	K	Joback Method
tc	1203.08	K	Joback Method
tf	597.90	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.75	J/mol×K	981.88	Joback Method
cpg	1110.54	J/mol×K	1018.75	Joback Method
cpg	1123.05	J/mol×K	1055.61	Joback Method
cpg	1134.38	J/mol×K	1092.48	Joback Method
cpg	1144.58	J/mol×K	1129.35	Joback Method
cpg	1153.74	J/mol×K	1166.22	Joback Method
cpg	1161.93	J/mol×K	1203.08	Joback Method

Sources

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=U377824&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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