Phthalic acid, decyl 2-trifluorobenzyl ester

Inchi: InChI=1S/C26H31F3O4/c1-2-3-4-5-6-7-8-13-18-32-24(30)21-15-10-11-16-22(21)25(31)3
InchiKey: OLDVWIPNYRDFCZ-UHFFFAOYSA-N
Formula: C26H31F3O4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 464.52

Physical Properties

Property code	Value	Unit	Source
gf	-675.83	kJ/mol	Joback Method
hf	-1216.53	kJ/mol	Joback Method
hfus	57.80	kJ/mol	Joback Method
hvap	93.91	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.360		Crippen Method
mcvol	349.870	ml/mol	McGowan Method
pc	1036.57	kPa	Joback Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	1004.76	K	Joback Method
tc	1230.18	K	Joback Method
tf	609.17	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.15	J/mol×K	1004.76	Joback Method
cpg	1171.17	J/mol×K	1042.33	Joback Method
cpg	1183.87	J/mol×K	1079.90	Joback Method
cpg	1195.34	J/mol×K	1117.47	Joback Method
cpg	1205.65	J/mol×K	1155.04	Joback Method
cpg	1214.90	J/mol×K	1192.61	Joback Method
cpg	1223.16	J/mol×K	1230.18	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=U377825&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