Phthalic acid, decyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C26H31F3O5/c1-2-3-4-5-6-7-8-11-18-32-24(30)22-12-9-10-13-23(22)25(31)33
InchiKey: ZCJRWHLBNFHPEE-UHFFFAOYSA-N
Formula: C26H31F3O5
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 480.52

Physical Properties

Property code	Value	Unit	Source
gf	-780.83	kJ/mol	Joback Method
hf	-1348.75	kJ/mol	Joback Method
hfus	58.99	kJ/mol	Joback Method
hvap	96.32	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	7.240		Crippen Method
mcvol	355.740	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	2884.00		NIST Webbook
rinpol	2884.00		NIST Webbook
tb	1027.18	K	Joback Method
tc	1257.70	K	Joback Method
tf	631.40	K	Joback Method
vc	1.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1183.99	J/mol×K	1027.18	Joback Method
cpg	1197.07	J/mol×K	1065.60	Joback Method
cpg	1208.65	J/mol×K	1104.02	Joback Method
cpg	1218.78	J/mol×K	1142.44	Joback Method
cpg	1227.53	J/mol×K	1180.86	Joback Method
cpg	1234.99	J/mol×K	1219.28	Joback Method
cpg	1241.21	J/mol×K	1257.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377692&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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