Terephthalic acid, propyl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C19H17F3O4/c1-2-11-25-17(23)14-5-7-15(8-6-14)18(24)26-12-13-3-9-16(10-4

InchiKey: YRHKKNLYSOTXGE-UHFFFAOYSA-N

Formula: C19H17F3O4

SMILES: CCCOC(=O)c1ccc(C(=O)OCc2ccc(C(F)(F)F)cc2)cc1

Mol. weight [g/mol]: 366.33

Physical Properties

Property code	Value	Unit	Source
gf	-734.77	kJ/mol	Joback Method
hf	-1072.05	kJ/mol	Joback Method
hfus	39.67	kJ/mol	Joback Method
hvap	78.33	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.629		Crippen Method
mcvol	251.240	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2712.00		NIST Webbook
rinpol	2712.00		NIST Webbook
tb	844.60	K	Joback Method
tc	1059.19	K	Joback Method
tf	530.28	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.86	J/mol×K	844.60	Joback Method
cpg	759.53	J/mol×K	880.37	Joback Method
cpg	771.09	J/mol×K	916.13	Joback Method
cpg	781.59	J/mol×K	951.90	Joback Method
cpg	791.09	J/mol×K	987.66	Joback Method
cpg	799.63	J/mol×K	1023.43	Joback Method
cpg	807.26	J/mol×K	1059.19	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=U383029&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