Terephthalic acid, ethyl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C18H15F3O4/c1-2-24-16(22)13-5-7-14(8-6-13)17(23)25-11-12-3-9-15(10-4-12

InchiKey: XLWXLFZQZVFFLV-UHFFFAOYSA-N

Formula: C18H15F3O4

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

Mol. weight [g/mol]: 352.30

Physical Properties

Property code	Value	Unit	Source
gf	-743.19	kJ/mol	Joback Method
hf	-1051.41	kJ/mol	Joback Method
hfus	37.08	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.239		Crippen Method
mcvol	237.150	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
rinpol	2607.00		NIST Webbook
rinpol	2607.00		NIST Webbook
tb	821.72	K	Joback Method
tc	1037.81	K	Joback Method
tf	519.01	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.13	J/mol×K	821.72	Joback Method
cpg	703.58	J/mol×K	857.74	Joback Method
cpg	714.94	J/mol×K	893.75	Joback Method
cpg	725.26	J/mol×K	929.77	Joback Method
cpg	734.58	J/mol×K	965.78	Joback Method
cpg	742.95	J/mol×K	1001.80	Joback Method
cpg	750.41	J/mol×K	1037.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383028&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