Terephthalic acid, heptyl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C23H25F3O4/c1-2-3-4-5-6-15-29-21(27)18-9-11-19(12-10-18)22(28)30-16-17-

InchiKey: UOGVEKBXDDWQGY-UHFFFAOYSA-N

Formula: C23H25F3O4

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

Mol. weight [g/mol]: 422.44

Physical Properties

Property code	Value	Unit	Source
gf	-701.09	kJ/mol	Joback Method
hf	-1154.61	kJ/mol	Joback Method
hfus	50.03	kJ/mol	Joback Method
hvap	87.23	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.190		Crippen Method
mcvol	307.600	ml/mol	McGowan Method
pc	1259.27	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook
tb	936.12	K	Joback Method
tc	1151.80	K	Joback Method
tf	575.36	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.54	J/mol×K	936.12	Joback Method
cpg	990.93	J/mol×K	972.07	Joback Method
cpg	1003.13	J/mol×K	1008.01	Joback Method
cpg	1014.19	J/mol×K	1043.96	Joback Method
cpg	1024.19	J/mol×K	1079.90	Joback Method
cpg	1033.18	J/mol×K	1115.85	Joback Method
cpg	1041.23	J/mol×K	1151.80	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=U383034&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