1,5-Pentanediol, O,O'-di(4-fluoro-2-trifluoromethylbenzoyl)-

Inchi: InChI=1S/C21H16F8O4/c22-12-4-6-14(16(10-12)20(24,25)26)18(30)32-8-2-1-3-9-33-19(

InchiKey: RLMWRIIYAMUENS-UHFFFAOYSA-N

Formula: C21H16F8O4

SMILES: O=C(OCCCCCOC(=O)c1ccc(F)cc1C(F)(F)F)c1ccc(F)cc1C(F)(F)F

Mol. weight [g/mol]: 484.34

Physical Properties

Property code	Value	Unit	Source
gf	-1708.40	kJ/mol	Joback Method
hf	-2125.57	kJ/mol	Joback Method
hfus	52.06	kJ/mol	Joback Method
hvap	78.72	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	6.187		Crippen Method
mcvol	288.270	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	2346.00		NIST Webbook
rinpol	2346.00		NIST Webbook
tb	893.44	K	Joback Method
tc	1096.10	K	Joback Method
tf	583.23	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.46	J/mol×K	893.44	Joback Method
cpg	906.83	J/mol×K	927.22	Joback Method
cpg	917.21	J/mol×K	960.99	Joback Method
cpg	926.68	J/mol×K	994.77	Joback Method
cpg	935.28	J/mol×K	1028.55	Joback Method
cpg	943.07	J/mol×K	1062.32	Joback Method
cpg	950.11	J/mol×K	1096.10	Joback Method

Sources

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=U343776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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