1,5-Pentanediol, O,O'-di(2,6-difluoro-3-methylbenzoyl)-

Inchi: InChI=1S/C21H20F4O4/c1-12-6-8-14(22)16(18(12)24)20(26)28-10-4-3-5-11-29-21(27)17

InchiKey: KSRKAKSFYPUGAZ-UHFFFAOYSA-N

Formula: C21H20F4O4

SMILES: Cc1ccc(F)c(C(=O)OCCCCCCOC(=O)c2c(F)ccc(C)c2F)c1F

Mol. weight [g/mol]: 412.37

Physical Properties

Property code	Value	Unit	Source
gf	-954.10	kJ/mol	Joback Method
hf	-1346.57	kJ/mol	Joback Method
hfus	53.79	kJ/mol	Joback Method
hvap	85.91	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	5.044		Crippen Method
mcvol	281.190	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	912.78	K	Joback Method
tc	1122.22	K	Joback Method
tf	601.07	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.32	J/mol×K	912.78	Joback Method
cpg	874.59	J/mol×K	947.69	Joback Method
cpg	885.68	J/mol×K	982.59	Joback Method
cpg	895.59	J/mol×K	1017.50	Joback Method
cpg	904.33	J/mol×K	1052.40	Joback Method
cpg	911.92	J/mol×K	1087.31	Joback Method
cpg	918.37	J/mol×K	1122.22	Joback Method

Sources

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=U343762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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