Glutaric acid, 1-(2,6-difluorophenyl)ethyl propyl ester

Inchi: InChI=1S/C16H20F2O4/c1-3-10-21-14(19)8-5-9-15(20)22-11(2)16-12(17)6-4-7-13(16)18

InchiKey: NNFXMLDPUUKUDO-UHFFFAOYSA-N

Formula: C16H20F2O4

SMILES: CCCOC(=O)CCCC(=O)OC(C)c1c(F)cccc1F

Mol. weight [g/mol]: 314.32

Physical Properties

Property code	Value	Unit	Source
gf	-682.91	kJ/mol	Joback Method
hf	-1047.08	kJ/mol	Joback Method
hfus	38.67	kJ/mol	Joback Method
hvap	71.10	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.692		Crippen Method
mcvol	230.960	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	752.80	K	Joback Method
tc	945.68	K	Joback Method
tf	452.04	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.63	J/mol×K	752.80	Joback Method
cpg	677.78	J/mol×K	784.95	Joback Method
cpg	691.04	J/mol×K	817.09	Joback Method
cpg	703.41	J/mol×K	849.24	Joback Method
cpg	714.91	J/mol×K	881.39	Joback Method
cpg	725.55	J/mol×K	913.53	Joback Method
cpg	735.32	J/mol×K	945.68	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=U377248&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