Glutaric acid, 3,4-difluorobenzyl hexyl ester

Inchi: InChI=1S/C18H24F2O4/c1-2-3-4-5-11-23-17(21)7-6-8-18(22)24-13-14-9-10-15(19)16(20
InchiKey: WZVMIAJZFLZNOT-UHFFFAOYSA-N
Formula: C18H24F2O4
SMILES: CCCCCCOC(=O)CCCC(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 342.38

Physical Properties

Property code	Value	Unit	Source
gf	-663.63	kJ/mol	Joback Method
hf	-1083.08	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	75.94	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.302		Crippen Method
mcvol	259.140	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	2473.00		NIST Webbook
rinpol	2473.00		NIST Webbook
tb	799.00	K	Joback Method
tc	990.08	K	Joback Method
tf	489.58	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.61	J/mol×K	799.00	Joback Method
cpg	790.29	J/mol×K	830.85	Joback Method
cpg	804.01	J/mol×K	862.69	Joback Method
cpg	816.79	J/mol×K	894.54	Joback Method
cpg	828.64	J/mol×K	926.39	Joback Method
cpg	839.57	J/mol×K	958.23	Joback Method
cpg	849.60	J/mol×K	990.08	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=U377638&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

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