Glutaric acid, 3,4-difluorobenzyl propyl ester

Inchi: InChI=1S/C15H18F2O4/c1-2-8-20-14(18)4-3-5-15(19)21-10-11-6-7-12(16)13(17)9-11/h6
InchiKey: MJAIAVMNAYWCPH-UHFFFAOYSA-N
Formula: C15H18F2O4
SMILES: CCCOC(=O)CCCC(=O)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 300.30

Physical Properties

Property code	Value	Unit	Source
gf	-688.89	kJ/mol	Joback Method
hf	-1021.16	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	69.26	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.131		Crippen Method
mcvol	216.870	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2147.00		NIST Webbook
tb	730.36	K	Joback Method
tc	921.52	K	Joback Method
tf	455.77	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.38	J/mol×K	730.36	Joback Method
cpg	621.95	J/mol×K	762.22	Joback Method
cpg	634.70	J/mol×K	794.08	Joback Method
cpg	646.64	J/mol×K	825.94	Joback Method
cpg	657.77	J/mol×K	857.80	Joback Method
cpg	668.10	J/mol×K	889.66	Joback Method
cpg	677.64	J/mol×K	921.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377633&Units=SI
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

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