Glutaric acid, butyl 3-fluorobenzyl ester

Inchi: InChI=1S/C16H21FO4/c1-2-3-10-20-15(18)8-5-9-16(19)21-12-13-6-4-7-14(17)11-13/h4,6
InchiKey: SYUXGIKWEWPUHB-UHFFFAOYSA-N
Formula: C16H21FO4
SMILES: CCCCOC(=O)CCCC(=O)OCc1cccc(F)c1
Mol. weight [g/mol]: 296.33

Physical Properties

Property code	Value	Unit	Source
gf	-476.03	kJ/mol	Joback Method
hf	-834.22	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	71.64	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.382		Crippen Method
mcvol	229.190	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2075.00		NIST Webbook
tb	748.99	K	Joback Method
tc	944.39	K	Joback Method
tf	453.93	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.18	J/mol×K	748.99	Joback Method
cpg	670.75	J/mol×K	781.56	Joback Method
cpg	684.40	J/mol×K	814.12	Joback Method
cpg	697.14	J/mol×K	846.69	Joback Method
cpg	708.99	J/mol×K	879.26	Joback Method
cpg	719.96	J/mol×K	911.83	Joback Method
cpg	730.06	J/mol×K	944.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376966&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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