Glutaric acid, heptyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C19H25F3O4/c1-2-3-4-5-6-12-25-17(23)8-7-9-18(24)26-13-14-15(20)10-11-16
InchiKey: RFUWDKMDHKLLDC-UHFFFAOYSA-N
Formula: C19H25F3O4
SMILES: CCCCCCCOC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 374.39

Physical Properties

Property code	Value	Unit	Source
gf	-859.65	kJ/mol	Joback Method
hf	-1311.30	kJ/mol	Joback Method
hfus	52.65	kJ/mol	Joback Method
hvap	78.01	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.831		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2346.00		NIST Webbook
rinpol	2346.00		NIST Webbook
tb	826.13	K	Joback Method
tc	1016.34	K	Joback Method
tf	513.96	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.99	J/mol×K	826.13	Joback Method
cpg	854.60	J/mol×K	857.83	Joback Method
cpg	868.22	J/mol×K	889.53	Joback Method
cpg	880.87	J/mol×K	921.23	Joback Method
cpg	892.56	J/mol×K	952.94	Joback Method
cpg	903.29	J/mol×K	984.64	Joback Method
cpg	913.09	J/mol×K	1016.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376900&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

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