Glutaric acid, propyl 2-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C16H19F3O4/c1-2-10-22-14(20)8-5-9-15(21)23-11-12-6-3-4-7-13(12)16(17,18
InchiKey: QOQHPEAZHDRCFM-UHFFFAOYSA-N
Formula: C16H19F3O4
SMILES: CCCOC(=O)CCCC(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
gf	-862.81	kJ/mol	Joback Method
hf	-1235.19	kJ/mol	Joback Method
hfus	38.25	kJ/mol	Joback Method
hvap	68.71	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.872		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1649.77	kPa	Joback Method
rinpol	2111.00		NIST Webbook
tb	744.30	K	Joback Method
tc	934.97	K	Joback Method
tf	457.53	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.84	J/mol×K	744.30	Joback Method
cpg	687.63	J/mol×K	776.08	Joback Method
cpg	700.53	J/mol×K	807.86	Joback Method
cpg	712.55	J/mol×K	839.63	Joback Method
cpg	723.74	J/mol×K	871.41	Joback Method
cpg	734.10	J/mol×K	903.19	Joback Method
cpg	743.68	J/mol×K	934.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377488&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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