Glutaric acid, monoamide, N-(3,5-di(trifluoromethyl)benzyl)-, ethyl ester

Inchi: InChI=1S/C16H17F6NO3/c1-2-26-14(25)5-3-4-13(24)23-9-10-6-11(15(17,18)19)8-12(7-1

InchiKey: XCZHWFWGIGFURX-UHFFFAOYSA-N

Formula: C16H17F6NO3

SMILES: CCOC(=O)CCCC(=O)NCc1cc(C(F)(F)F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 385.30

Physical Properties

Property code	Value	Unit	Source
gf	-1259.64	kJ/mol	Joback Method
hf	-1658.05	kJ/mol	Joback Method
hfus	43.60	kJ/mol	Joback Method
hvap	69.65	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.074		Crippen Method
mcvol	242.150	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook
tb	771.61	K	Joback Method
tc	957.37	K	Joback Method
tf	504.67	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.79	J/mol×K	771.61	Joback Method
cpg	738.10	J/mol×K	802.57	Joback Method
cpg	749.57	J/mol×K	833.53	Joback Method
cpg	760.26	J/mol×K	864.49	Joback Method
cpg	770.21	J/mol×K	895.45	Joback Method
cpg	779.46	J/mol×K	926.41	Joback Method
cpg	788.07	J/mol×K	957.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360763&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