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

Inchi: InChI=1S/C26H37F6NO3/c1-2-3-4-5-6-7-8-9-10-11-15-36-24(35)14-12-13-23(34)33-19-2
InchiKey: NGNKPQYCJSKTJO-UHFFFAOYSA-N
Formula: C26H37F6NO3
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)NCc1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 525.57

Physical Properties

Property code	Value	Unit	Source
gf	-1175.44	kJ/mol	Joback Method
hf	-1864.45	kJ/mol	Joback Method
hfus	69.50	kJ/mol	Joback Method
hvap	91.91	kJ/mol	Joback Method
log10ws	-9.50		Crippen Method
logp	7.975		Crippen Method
mcvol	383.050	ml/mol	McGowan Method
pc	805.70	kPa	Joback Method
rinpol	2859.00		NIST Webbook
rinpol	2859.00		NIST Webbook
tb	1000.41	K	Joback Method
tc	1235.69	K	Joback Method
tf	617.37	K	Joback Method
vc	1.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.06	J/mol×K	1000.41	Joback Method
cpg	1332.49	J/mol×K	1039.62	Joback Method
cpg	1348.63	J/mol×K	1078.84	Joback Method
cpg	1363.63	J/mol×K	1118.05	Joback Method
cpg	1377.63	J/mol×K	1157.26	Joback Method
cpg	1390.76	J/mol×K	1196.47	Joback Method
cpg	1403.18	J/mol×K	1235.69	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360773&Units=SI

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