

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

InChI:
InChIKey:

InChI=1S/C29H43F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-39-27(38)17-15-16-26(3)

CPTQNBHCAQTPIC-UHFFFAOYSA-N

Formula:

C29H43F6NO3

SMILES:

CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)NCc1cc(C(F)(F)F)cc(C(F)(F)F)c1

Mol. weight [g/mol]:

567.65

Physical Properties

Property code	Value	Unit	Source
gf	-1150.18	kJ/mol	Joback Method
hf	-1926.37	kJ/mol	Joback Method
hfus	77.27	kJ/mol	Joback Method
hvap	98.59	kJ/mol	Joback Method
log10ws	-10.76		Crippen Method
logp	9.145		Crippen Method
mcvol	425.320	ml/mol	McGowan Method
pc	688.53	kPa	Joback Method
rinpol	3165.00		NIST Webbook
rinpol	3165.00		NIST Webbook
tb	1069.05	K	Joback Method
tc	1341.75	K	Joback Method
tf	651.18	K	Joback Method
vc	1.702	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1503.77	J/molxK	1069.05	Joback Method
cpg	1523.93	J/molxK	1114.50	Joback Method
cpg	1542.55	J/molxK	1159.95	Joback Method
cpg	1559.86	J/molxK	1205.40	Joback Method
cpg	1576.11	J/molxK	1250.85	Joback Method
cpg	1591.54	J/molxK	1296.30	Joback Method
cpg	1606.38	J/molxK	1341.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360775&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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