Glutaric acid, octadecyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C31H49F3O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-25-37-29(35)19-18

InchiKey: MZDGMXHGWNXOEG-UHFFFAOYSA-N

Formula: C31H49F3O5

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 558.71

Physical Properties

Property code	Value	Unit	Source
gf	-841.51	kJ/mol	Joback Method
hf	-1677.01	kJ/mol	Joback Method
hfus	78.29	kJ/mol	Joback Method
hvap	104.51	kJ/mol	Joback Method
log10ws	-10.98		Crippen Method
logp	9.603		Crippen Method
mcvol	449.950	ml/mol	McGowan Method
pc	651.10	kPa	Joback Method
rinpol	3483.00		NIST Webbook
rinpol	3483.00		NIST Webbook
tb	1109.92	K	Joback Method
tc	1400.75	K	Joback Method
tf	648.81	K	Joback Method
vc	1.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1607.48	J/mol×K	1109.92	Joback Method
cpg	1626.67	J/mol×K	1158.39	Joback Method
cpg	1643.23	J/mol×K	1206.86	Joback Method
cpg	1657.35	J/mol×K	1255.33	Joback Method
cpg	1669.21	J/mol×K	1303.81	Joback Method
cpg	1678.99	J/mol×K	1352.28	Joback Method
cpg	1686.87	J/mol×K	1400.75	Joback Method

Sources

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=U377349&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/97-214-7/Glutaric-acid-octadecyl-4-trifluoromethoxy-benzyl-ester.pdf
Generated by Cheméo on 2024-05-02 07:34:13.337778544 +0000 UTC m=+16924502.258355861.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.