Glutaric acid, hexadecyl 1-phenyl-2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C29H45F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-24-35-26(33)22-19-23-27

InchiKey: VIDQGRURRMJEDZ-UHFFFAOYSA-N

Formula: C29H45F3O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 514.66

Physical Properties

Property code	Value	Unit	Source
gf	-746.16	kJ/mol	Joback Method
hf	-1497.32	kJ/mol	Joback Method
hfus	68.78	kJ/mol	Joback Method
hvap	96.60	kJ/mol	Joback Method
log10ws	-9.91		Crippen Method
logp	9.028		Crippen Method
mcvol	415.900	ml/mol	McGowan Method
pc	735.62	kPa	Joback Method
rinpol	3199.00		NIST Webbook
rinpol	3199.00		NIST Webbook
tb	1036.32	K	Joback Method
tc	1282.35	K	Joback Method
tf	576.52	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1453.49	J/mol×K	1036.32	Joback Method
cpg	1472.40	J/mol×K	1077.33	Joback Method
cpg	1489.56	J/mol×K	1118.33	Joback Method
cpg	1505.13	J/mol×K	1159.34	Joback Method
cpg	1519.22	J/mol×K	1200.34	Joback Method
cpg	1531.98	J/mol×K	1241.35	Joback Method
cpg	1543.53	J/mol×K	1282.35	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=U377378&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