Glutaric acid, 2,2,3,3,4,4,4-heptafluorobutyl hexadecyl ester

Inchi: InChI=1S/C25H41F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-35-21(33)17-16-18-22

InchiKey: RFVVUHJYXOSGHK-UHFFFAOYSA-N

Formula: C25H41F7O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 538.58

Physical Properties

Property code	Value	Unit	Source
gf	-1663.37	kJ/mol	Joback Method
hf	-2447.95	kJ/mol	Joback Method
hfus	65.40	kJ/mol	Joback Method
hvap	79.95	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	8.557		Crippen Method
mcvol	390.380	ml/mol	McGowan Method
pc	698.39	kPa	Joback Method
rinpol	2775.00		NIST Webbook
tb	909.18	K	Joback Method
tc	1126.36	K	Joback Method
tf	527.22	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1330.02	J/mol×K	909.18	Joback Method
cpg	1350.20	J/mol×K	945.38	Joback Method
cpg	1368.98	J/mol×K	981.57	Joback Method
cpg	1386.48	J/mol×K	1017.77	Joback Method
cpg	1402.81	J/mol×K	1053.97	Joback Method
cpg	1418.10	J/mol×K	1090.17	Joback Method
cpg	1432.46	J/mol×K	1126.36	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=U377561&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