Glutaric acid, hexadecyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C26H42F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-37-21(35)17-16-18-22

InchiKey: XJUZVLNKBGNWGD-UHFFFAOYSA-N

Formula: C26H42F8O4

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

Mol. weight [g/mol]: 570.60

Physical Properties

Property code	Value	Unit	Source
gf	-1852.20	kJ/mol	Joback Method
hf	-2669.98	kJ/mol	Joback Method
hfus	67.54	kJ/mol	Joback Method
hvap	80.97	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	8.895		Crippen Method
mcvol	406.240	ml/mol	McGowan Method
pc	651.77	kPa	Joback Method
rinpol	2747.00		NIST Webbook
rinpol	2747.00		NIST Webbook
tb	930.89	K	Joback Method
tc	1162.11	K	Joback Method
tf	524.08	K	Joback Method
vc	1.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1400.30	J/mol×K	930.89	Joback Method
cpg	1421.52	J/mol×K	969.43	Joback Method
cpg	1441.18	J/mol×K	1007.96	Joback Method
cpg	1459.41	J/mol×K	1046.50	Joback Method
cpg	1476.37	J/mol×K	1085.04	Joback Method
cpg	1492.20	J/mol×K	1123.58	Joback Method
cpg	1507.05	J/mol×K	1162.11	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=U359691&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