Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 8-chlorooctyl ester

Inchi: InChI=1S/C18H25ClF8O4/c19-10-5-3-1-2-4-6-11-30-13(28)8-7-9-14(29)31-12-16(22,23)1

InchiKey: AWBDYWQBWQNEFO-UHFFFAOYSA-N

Formula: C18H25ClF8O4

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

Mol. weight [g/mol]: 492.83

Physical Properties

Property code	Value	Unit	Source
gf	-1931.49	kJ/mol	Joback Method
hf	-2520.60	kJ/mol	Joback Method
hfus	51.02	kJ/mol	Joback Method
hvap	67.55	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.994		Crippen Method
mcvol	305.760	ml/mol	McGowan Method
pc	985.16	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	785.28	K	Joback Method
tc	961.53	K	Joback Method
tf	463.84	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.06	J/mol×K	785.28	Joback Method
cpg	960.49	J/mol×K	814.65	Joback Method
cpg	974.01	J/mol×K	844.03	Joback Method
cpg	986.68	J/mol×K	873.40	Joback Method
cpg	998.55	J/mol×K	902.78	Joback Method
cpg	1009.67	J/mol×K	932.15	Joback Method
cpg	1020.09	J/mol×K	961.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393457&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
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