

Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 10-chlorodecyl ester

Inchi:	InChI=1S/C20H29ClF8O4/c21-12-7-5-3-1-2-4-6-8-13-32-15(30)10-9-11-16(31)33-14-18(
InchiKey:	ONGMNPBWYPPFRD-UHFFFAOYSA-N
Formula:	C20H29ClF8O4
SMILES:	O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)OCCCCCCCCCCI
Mol. weight [g/mol]:	520.88

Physical Properties

Property code	Value	Unit	Source
gf	-1914.65	kJ/mol	Joback Method
hf	-2561.88	kJ/mol	Joback Method
hfus	56.20	kJ/mol	Joback Method
hvap	72.00	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	6.774		Crippen Method
mcvol	333.940	ml/mol	McGowan Method
pc	876.36	kPa	Joback Method
rinqol	2406.00		NIST Webbook
tb	831.04	K	Joback Method
tc	1018.37	K	Joback Method
tf	486.38	K	Joback Method
vc	1.357	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.74	J/molxK	831.04	Joback Method
cpg	1078.35	J/molxK	862.26	Joback Method
cpg	1092.94	J/molxK	893.48	Joback Method
cpg	1106.58	J/molxK	924.70	Joback Method
cpg	1119.33	J/molxK	955.93	Joback Method
cpg	1131.27	J/molxK	987.15	Joback Method
cpg	1142.46	J/molxK	1018.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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