

Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,4-dichloro-1-naphthyl ester

Inchi: InChI=1S/C20H14Cl2F8O4/c21-12-8-13(22)16(11-5-2-1-4-10(11)12)34-15(32)7-3-6-14(3

InchiKey: AHCTWZKDGTVCCO-UHFFFAOYSA-N

Formula: C₂₀H₁₄Cl₂F₈O₄

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 541.22

Physical Properties

Property code	Value	Unit	Source
gf	-1736.41	kJ/mol	Joback Method
hf	-2184.43	kJ/mol	Joback Method
hfus	50.29	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	6.936		Crippen Method
mcvol	302.960	ml/mol	McGowan Method
pc	1202.29	kPa	Joback Method
rinpol	2672.00		NIST Webbook
rinpol	2672.00		NIST Webbook
tb	929.07	K	Joback Method
tc	1139.51	K	Joback Method
tf	612.98	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.44	J/mol×K	929.07	Joback Method
cpg	916.37	J/mol×K	964.14	Joback Method
cpg	925.60	J/mol×K	999.22	Joback Method
cpg	934.26	J/mol×K	1034.29	Joback Method
cpg	942.45	J/mol×K	1069.36	Joback Method
cpg	950.26	J/mol×K	1104.44	Joback Method
cpg	957.81	J/mol×K	1139.51	Joback Method

Sources

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=U392015&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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