

Glutaric acid, heptyl 2,3,4,5-tetrafluorobenzyl ester

Inchi:	InChI=1S/C19H24F4O4/c1-2-3-4-5-6-10-26-15(24)8-7-9-16(25)27-12-13-11-14(20)18(22)
InchiKey:	OKJMDJXSZUDVQY-UHFFFAOYSA-N
Formula:	C19H24F4O4
SMILES:	CCCCCCCOC(=O)CCCC(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]:	392.39

Physical Properties

Property code	Value	Unit	Source
gf	-1064.09	kJ/mol	Joback Method
hf	-1518.88	kJ/mol	Joback Method
hfus	55.34	kJ/mol	Joback Method
hvap	77.86	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	4.970		Crippen Method
mcvol	276.770	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpola	2337.00		NIST Webbook
rinpola	2337.00		NIST Webbook
tb	830.38	K	Joback Method
tc	1019.22	K	Joback Method
tf	527.07	K	Joback Method
vc	1.111	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.65	J/molxK	830.38	Joback Method
cpg	860.92	J/molxK	861.85	Joback Method
cpg	874.21	J/molxK	893.33	Joback Method
cpg	886.55	J/molxK	924.80	Joback Method
cpg	897.94	J/molxK	956.28	Joback Method
cpg	908.38	J/molxK	987.75	Joback Method
cpg	917.88	J/molxK	1019.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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