

Glutaric acid, 2,2,2-trifluoroethyl heptadecyl ester

Inchi:	InChI=1S/C24H43F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-30-22(28)18-17-19
InchiKey:	MSJWAKIIAGAWLA-UHFFFAOYSA-N
Formula:	C24H43F3O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]:	452.59

Physical Properties

Property code	Value	Unit	Source
gf	-898.23	kJ/mol	Joback Method
hf	-1625.37	kJ/mol	Joback Method
hfus	65.32	kJ/mol	Joback Method
hvap	83.58	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.677		Crippen Method
mvol	369.210	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
rinpol	2599.00		NIST Webbook
rinpol	2599.00		NIST Webbook
tb	895.68	K	Joback Method
tc	1101.29	K	Joback Method
tf	508.75	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.83	J/mol×K	895.68	Joback Method
cpg	1258.74	J/mol×K	929.95	Joback Method
cpg	1277.28	J/mol×K	964.22	Joback Method
cpg	1294.50	J/mol×K	998.48	Joback Method
cpg	1310.45	J/mol×K	1032.75	Joback Method
cpg	1325.20	J/mol×K	1067.02	Joback Method
cpg	1338.79	J/mol×K	1101.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380524&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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