

Glutaric acid, dodecyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C19H33Cl3O4/c1-2-3-4-5-6-7-8-9-10-11-15-25-17(23)13-12-14-18(24)26-16-19
InchiKey:	OQAVDQVRXJQCBU-UHFFFAOYSA-N
Formula:	C19H33Cl3O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	431.82

Physical Properties

Property code	Value	Unit	Source
gf	-391.69	kJ/mol	Joback Method
hf	-981.06	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	88.06	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.534		Crippen Method
mcvol	330.170	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2736.00		NIST Webbook
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tb	895.76	K	Joback Method
tc	1098.51	K	Joback Method
tf	540.39	K	Joback Method
vc	1.284	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.08	J/molxK	895.76	Joback Method
cpg	1013.04	J/molxK	929.55	Joback Method
cpg	1026.95	J/molxK	963.34	Joback Method
cpg	1039.83	J/molxK	997.14	Joback Method
cpg	1051.74	J/molxK	1030.93	Joback Method
cpg	1062.71	J/molxK	1064.72	Joback Method
cpg	1072.80	J/molxK	1098.51	Joback Method
dvisc	0.0004095	Paxs	540.39	Joback Method

dvisc	0.0002124	Paxs	599.62	Joback Method
dvisc	0.0001240	Paxs	658.85	Joback Method
dvisc	0.0000791	Paxs	718.08	Joback Method
dvisc	0.0000540	Paxs	777.30	Joback Method
dvisc	0.0000390	Paxs	836.53	Joback Method
dvisc	0.0000293	Paxs	895.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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

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