

Glutaric acid, 8-chlorooctyl hept-4-yl ester

Inchi:	InChI=1S/C20H37ClO4/c1-3-12-18(13-4-2)25-20(23)15-11-14-19(22)24-17-10-8-6-5-7-9
InchiKey:	VCAOIPKVKONHQD-UHFFFAOYSA-N
Formula:	C20H37ClO4
SMILES:	CCCC(CCC)OC(=O)CCCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	376.96

Physical Properties

Property code	Value	Unit	Source
gf	-364.69	kJ/mol	Joback Method
hf	-966.75	kJ/mol	Joback Method
hfus	53.80	kJ/mol	Joback Method
hvap	82.42	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.791		Crippen Method
mvol	319.780	ml/mol	McGowan Method
pc	1057.57	kPa	Joback Method
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook
tb	846.57	K	Joback Method
tc	1037.93	K	Joback Method
tf	474.40	K	Joback Method
vc	1.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.30	J/molxK	846.57	Joback Method
cpg	1018.70	J/molxK	878.46	Joback Method
cpg	1034.98	J/molxK	910.36	Joback Method
cpg	1050.18	J/molxK	942.25	Joback Method
cpg	1064.31	J/molxK	974.15	Joback Method
cpg	1077.39	J/molxK	1006.04	Joback Method
cpg	1089.45	J/molxK	1037.93	Joback Method
dvisc	0.0007660	Paxs	474.40	Joback Method

dvisc	0.0003564	Paxs	536.43	Joback Method
dvisc	0.0001943	Paxs	598.46	Joback Method
dvisc	0.0001187	Paxs	660.48	Joback Method
dvisc	0.0000789	Paxs	722.51	Joback Method
dvisc	0.0000560	Paxs	784.54	Joback Method
dvisc	0.0000418	Paxs	846.57	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U392526&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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