

Glutaric acid, 8-chlorooctyl heptyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-362.25	kJ/mol	Joback Method
hf	-961.47	kJ/mol	Joback Method
hfus	57.33	kJ/mol	Joback Method
hvap	82.81	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.793		Crippen Method
mvol	319.780	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	2719.00		NIST Webbook
tb	847.01	K	Joback Method
tc	1037.90	K	Joback Method
tf	489.40	K	Joback Method
vc	1.252	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.82	J/molxK	847.01	Joback Method
cpg	1076.89	J/molxK	1006.09	Joback Method
cpg	1063.78	J/molxK	974.27	Joback Method
cpg	1049.64	J/molxK	942.46	Joback Method
cpg	1034.44	J/molxK	910.64	Joback Method
cpg	1018.18	J/molxK	878.83	Joback Method
cpg	1088.99	J/molxK	1037.90	Joback Method
dvisc	0.0000456	Paxs	847.01	Joback Method
dvisc	0.0000601	Paxs	787.41	Joback Method

dvisc	0.0000830	Paxs	727.81	Joback Method
dvisc	0.0001214	Paxs	668.20	Joback Method
dvisc	0.0001913	Paxs	608.60	Joback Method
dvisc	0.0003326	Paxs	549.00	Joback Method
dvisc	0.0006619	Paxs	489.40	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359588&Units=SI

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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