Glutaric acid, hex-4-yn-3-yl 10-chlorodecyl ester

Inchi: InChI=1S/C21H35ClO4/c1-3-14-19(4-2)26-21(24)16-13-15-20(23)25-18-12-10-8-6-5-7-9-

InchiKey: XADLJHUICPGKFR-UHFFFAOYSA-N

Formula: C21H35ClO4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCCCCCCCCCCCCl

Mol. weight [g/mol]: 386.95

Physical Properties

Property code	Value	Unit	Source
gf	-153.47	kJ/mol	Joback Method
hf	-715.09	kJ/mol	Joback Method
hfus	59.52	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.405		Crippen Method
mcvol	325.270	ml/mol	McGowan Method
pc	1103.01	kPa	Joback Method
rinpol	2716.00		NIST Webbook
rinpol	2716.00		NIST Webbook
tb	878.45	K	Joback Method
tc	1078.67	K	Joback Method
tf	591.77	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.14	J/mol×K	878.45	Joback Method
cpg	1026.85	J/mol×K	911.82	Joback Method
cpg	1042.39	J/mol×K	945.19	Joback Method
cpg	1056.80	J/mol×K	978.56	Joback Method
cpg	1070.09	J/mol×K	1011.93	Joback Method
cpg	1082.28	J/mol×K	1045.30	Joback Method
cpg	1093.40	J/mol×K	1078.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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