TRIPENTYL CITRATE

Inchi: InChI=1S/C21H38O7/c1-4-7-10-13-26-18(22)16-21(25,20(24)28-15-12-9-6-3)17-19(23)2
InchiKey: DXRFOGXSSDRZFP-UHFFFAOYSA-N
Formula: C21H38O7
SMILES: CCCCCOC(=O)CC(O)(CC(=O)OCCCCC)C(=O)OCCCCC
Mol. weight [g/mol]: 402.53

Physical Properties

Property code	Value	Unit	Source
af	1.2399		Cheméo Relay (1.0)
hf	-1578.65	kJ/mol	Cheméo Relay (1.0)
hfus	55.18	kJ/mol	Joback Method
hvap	103.75	kJ/mol	Cheméo Relay (1.0)
ie	9.52	eV	Cheméo Relay (1.0)
log10ws	-3.84		Cheméo Relay (1.0)
logp	3.698		Crippen Method
mcvol	334.940	ml/mol	McGowan Method
pc	1122.31	kPa	Joback Method
tb	639.06	K	Cheméo Relay (1.0)
tc	823.59	K	Cheméo Relay (1.0)
tf	289.61	K	Cheméo Relay (1.0)
vc	1.264	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1144.49	J/mol×K	997.70	Joback Method
cpg	1159.51	J/mol×K	1036.21	Joback Method
cpg	1172.95	J/mol×K	1074.72	Joback Method
cpg	1184.86	J/mol×K	1113.23	Joback Method
cpg	1195.29	J/mol×K	1151.73	Joback Method
cpg	1204.27	J/mol×K	1190.24	Joback Method
cpg	1211.85	J/mol×K	1228.75	Joback Method
dvisc	0.0000938	Pa×s	606.15	Joback Method
dvisc	0.0000398	Pa×s	671.41	Joback Method

dvisc	0.0000196	Pa×s	736.67	Joback Method
dvisc	0.0000109	Pa×s	801.92	Joback Method
dvisc	0.0000066	Pa×s	867.18	Joback Method
dvisc	0.0000043	Pa×s	932.44	Joback Method
dvisc	0.0000029	Pa×s	997.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70289348&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume