Glutaric acid, 2-(2-chlorophenyl)ethyl pentyl ester

Inchi: InChI=1S/C18H25ClO4/c1-2-3-6-13-22-17(20)10-7-11-18(21)23-14-12-15-8-4-5-9-16(15)

InchiKey: OADQUUCHJAMNAX-UHFFFAOYSA-N

Formula: C18H25ClO4

SMILES: CCCCCOC(=O)CCCC(=O)OCCc1ccccc1Cl

Mol. weight [g/mol]: 340.84

Physical Properties

Property code	Value	Unit	Source
af	0.9030		Cheméo Relay (1.0)
hf	-823.13	kJ/mol	Cheméo Relay (1.0)
hfus	48.96	kJ/mol	Joback Method
hvap	101.97	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.78		Cheméo Relay (1.0)
logp	4.329		Crippen Method
mcvol	267.840	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2496.00		NIST Webbook
rinpol	2496.00		NIST Webbook
tb	640.87	K	Cheméo Relay (1.0)
tc	835.61	K	Cheméo Relay (1.0)
tf	281.07	K	Cheméo Relay (1.0)
vc	0.996	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	3.06290e+01
Coeff. B	1.47262e+00
Coeff. C	-7.50760e-04
Coeff. D	9.84000e-08
Coeff. E	0.00000e+00

Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.36106e+01
Coeff. B	2.93824e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	446.14
Temperature range (K), max.	697.48

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U377269&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

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

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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